ErbB4 CO-CRYSTAL

BACKGROUND OF THE INVENTION

The present invention relates to the crystal structure of the ErbB4 kinase domain (ErbB4K), specifically the ErbB4K in liganded form as well as methods of using the same in the discovery of ErbB4 inhibitors and in the treatment of diseases mediated by inappropriate ErbB4 activity.

Abberant protein tyrosine kinase (PTK) activity has been implicated in a variety of disorders including psoriasis, rheumatoid arthritis, bronchitis, as well as cancer. Development of effective treatments for such disorders is a constant and ongoing enterprise in the medical field. The ErbB family of PTKs, which includes c-ErbB-2, EGFR, and ErbB-4, is one group of PTKs that has attracted interest as a therapeutic target. Currently, of special interest, is the role of ErbB family PTKs in hyperproliferative disorders, particularly human malignancies. Consequently, inhibition of ErbB family PTKs should provide for disorders characterized by aberrant ErbB family PTK activity. The biological role of ErbB family PTKs and their implication in various disease states is discussed, for instance in US patent 5,773,476; International patent application WO99/35146; M.C Hung et al, Seminars in Oncology, 26: 4, Suppl. 12 (August) 1999, 51-59; Ulrich et al, Cell, 61:203-212, April 20, 1990; Modjtahedi et al, Int'l J. of Oncology, 13: 335-342, 1998; and J.R. Woodburn, Pharmacol. Ther., 82: 2-3, 241-250, 1999.

Polypeptides, including ErbB4, have a three-dimensional structure determined by the primary amino acid sequence and the environment surrounding the polypeptide. This three-dimensional structure establishes the polypeptide's activity, stability, binding affinity, binding specificity, and other biochemical attributes. Thus, knowledge of a protein's three-dimensional

structure can provide much guidance in designing agents that mimic, inhibit, or improve its biological activity in soluble or membrane bound forms.

The three-dimensional structure of a polypepetide can be determined in a number of ways. Many of the most precise methods employ X-ray crystallography (See, e.g., Van Holde, (1971) Physical Biochemistry, Prentice-Hall, N. J., 221-239). This technique relies on the ability of crystalline lattices to diffract X-rays or other forms of radiation. Diffraction experiments suitable for determining the three-dimensional structure of macromolecules typically require high-quality crystals. Since such crystals have been unavailable for ErbB4, a three-dimensional structure of ErbB4 has proven difficult to elucidate.

The present inventors have developed such crystals and have now determined the crystal structure of the nonphosphorylated human ErbB4K complexed with an irreversible inhibitor to 2.5 Å resolution. Such a crystal structure is useful in discovering compounds suitable for inhibiting ErbB4 and for treating diseases characterized by aberrant ErbB4 activity.

BRIEF SUMMARY OF THE INVENTION

In one aspect of the present invention, there is provided an ErbB4 kinase domain in liganded crystalline form, comprising the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2.

In a second aspect of the present invention, there is provided a method of ErbB4 inhibitor design, comprising:

generating a three dimensional computer model which represents ErbB4 kinase domain in liganded form, said kinase domain described by the

amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2;

evaluating compounds as potential ErbB4 inhibitors using said model; and

selecting compounds for further testing based on said evaluation.

In a third aspect of the present invention, there is provided a method of ErbB4 inhibitor design, comprising:

generating a three dimensional computer model which represents an ErbB4 kinase domain in liganded form, said kinase domain described by the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2;

evaluating compounds as potential ErbB4 inhibitors using said model; wherein said evaluation comprises identifying compounds capable of at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface; and

selecting compounds for further testing based on said evaluation.

In a fourth aspect of the present invention, there is provided a method of ErbB4 inhibitor design, comprising:

generating a three dimensional computer model which represents a ErbB4 kinase domain in liganded form, said kinase domain described by the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2;

evaluating compounds as potential ErbB4 inhibitors using said model; wherein said evaluation comprises identifying compounds capable of at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues 796, 797, 798, 799, and 800;

(ii) one or more interactions with amino acid residues 724, 749, and 850;

(iii) one or more interactions with amino acid residues 848, 860, 803, 847, 732, and 725;

(iv) one or more interactions with amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862; and

(v) one or more interactions with residues 801, 802, 803, 806, and 810; and

selecting compounds for further testing based on said evaluation.

In a fifth aspect of the present invention, there is provided a method of treating a disorder characterized by inappropriate ErbB4 activity in a mammal, comprising: administering to said mammal a therapeutically effective amount

of a compound that can form a complex with an ErbB4 kinase domain thereby resulting in a ErbB4 kinase domain in liganded form, said kinase domain in liganded form being described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2, wherein said complex is characterized by at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface.

In a sixth aspect of the present invention, there is provided a method of inhibiting ErbB4 in a mammal, comprising: administering to said mammal a therapeutically effective amount of a compound that can form a complex with a ErbB4 kinase domain thereby resulting in an ErbB4 kinase domain in liganded form, said kinase domain in liganded form being described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2, wherein said complex is characterized by at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface.

In a seventh aspect of the present invention, there is provided an ErbB4 kinase domain/inhibitor complex, comprising: an ErbB4 kinase domain form being described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2 and a compound that can form a complex with the ErbB4 kinase domain said complex is characterized by at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 depicts the structure of two thienopyrimidine inhibitors before reaction with the protein.

Figure 2 depicts a ribbon representation of the ErbB4K complexed with an irreversible inhibitor. A loop that is disordered in the crystal structure is shown as a dashed line. The figure was prepared with RIBBONS.

Figure 3 depicts the binding of a thienopyrimidine inhibitor in the ATP binding site of ErbB4K. The inhibitor is highlighted with thick black lines. The hydrogen bond between the inhibitor and the backbone NH of Met799 is shown as a grey dashed line. The covalent bond between the inhibitor and Cys803 is shown as a black dashed line. The figure was created with QUANTA.

DETAILED DESCRIPTION OF THE INVENTION

Table 1 is a table summarizing the crystal and data statistics obtained from ErbB4K crystal forms. Data on the unit cell is presented, including data on the crystal space group, unit cell dimensions, molecules per asymmetric cell and crystal resolution.

Table 2 is a table of the atomic structure coordinate data obtained from X-ray diffraction from the liganded ErbB4K crystal form.

As used herein, the term "effective amount" means that amount of a drug or pharmaceutical agent that will elicit the biological or medical response of a tissue, system, animal or human that is being sought, for instance, by a researcher or clinician. Furthermore, the term "therapeutically effective amount" means any amount which, as compared to a corresponding subject who has not received such amount, results in improved treatment, healing, prevention, or amelioration of a disease, disorder, or side effect, or a decrease in the rate of advancement of a disease or disorder. The term also

includes within its scope amounts effective to enhance normal physiological function.

As used herein, the term "mutation" carries its traditional connotation and means a change, inherited, naturally occurring or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art.

As used herein, the term "labeled" means the attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be standard in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length. Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

As used herein, the term "transcription" means a cellular process involving the interaction of an RNA polymerase with a gene that directs the expression as RNA of the structural information present in the coding sequences of the gene. The process includes, but is not limited to, the following steps: (a) the transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of the transcript, (h) transcript editing, and (i) stabilizing the transcript.

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced from RNA.

As used herein, the term "transcription factor" means a cytoplasmic or nuclear protein which binds to a gene, or binds to an RNA transcript of such gene, or binds to another protein which binds to such gene or such RNA transcript or another protein which in turn binds to such gene or such RNA transcript, so as to thereby modulate expression of the gene. Such modulation can additionally be achieved by other mechanisms; the essence of "transcription factor for a gene" is that the level of transcription of the gene is altered in some way.

As used herein, the term "hybridization" means the binding of a probe molecule, a molecule to which a detectable moiety has been bound, to a target sample.

As used herein, the term "detecting" means confirming the presence of a target entity by observing the occurrence of a detectable signal, such as a radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

As used herein, the term "sequencing" means determining the ordered linear sequence of nucleic acids or amino acids of a DNA or protein target sample, using conventional manual or automated laboratory techniques.

As used herein, the term "isolated" means for example oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to other molecule types including polypeptides, in which case the polypeptide will be substantially free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

As used herein, the term "substantially pure" means that the polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is associated in its natural state, and those molecules used in the isolation procedure. The term "substantially free" means that the sample is at least 50%, preferably at least 70%, more preferably 80% and most preferably 90% free of the materials and compounds with which it is associated in nature.

As used herein, the term "primer" means a sequence comprising two or more deoxyribonucleotides or ribonucleotides, preferably more than three, and more preferably more than eight and most preferably at least about 20 nucleotides of an exonic or intronic region. Such oligonucleotides are preferably between ten and thirty bases in length.

As used herein, the term "DNA segment" means a DNA molecule that has been isolated free of total genomic DNA of a particular species. For example, a DNA segment encoding a erbB4 or erbB4K polypeptide refers to a DNA segment that encodes SEQ ID NO: 1 yet is isolated away from, or purified free from, total genomic DNA of a source species, such as *Homo sapiens*. Included within the term "DNA segment" are DNA segments and smaller fragments of such segments, and also recombinant vectors, including, for example, plasmids, cosmids, phages, viruses, and the like.

As used herein, the phrase "enhancer-promoter" means a composite unit that contains both enhancer and promoter elements. An enhancer-promoter is operatively linked to a coding sequence that encodes at least one gene product.

As used herein, the phrase "operatively linked" means that an enhancer-promoter is connected to a coding sequence in such a way that the transcription of that coding sequence is controlled and regulated by that enhancer-promoter. Techniques for operatively linking an enhancer-promoter to a coding sequence are well known in the art; the precise orientation and location relative to a coding sequence of interest is dependent, *inter alia*, upon the specific nature of the enhancer-promoter.

As used herein, the term "inhibitor candidate" means a substance that is believed to interact with another moiety, for example a given ligand that is believed to interact to at least partially inhibit the activity of a complete enzyme or enzyme polypeptide, or fragment thereof, and which can be subsequently evaluated for such an interaction and activity inhibition. In a like manner, the term "ErbB4 inhibitor candidate" means a substance that is believed to interact with another moiety, for example a given ligand that is believed to interact to at least partially inhibit the activity of a complete ErbB4 or ErbB4 polypeptide, or fragment thereof, and which can be subsequently evaluated for such an interaction and activity inhibition. Representative candidate compounds or substrates include xenobiotics such as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as steroids, fatty acids and prostaglandins. Other examples of candidate substances that can be investigated using the methods of the present invention include, but are not restricted to, agonists and antagonists of a ErbB4 or ErbB4 polypeptide, toxins and venoms, viral epitopes, hormones (e.g., opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

As used herein, the term "modified" means an alteration from an

entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

As used herein, the term "interaction" means any relationship between atoms or molecules whereby atomic and/or molecular conditions or forces exist which promote binding equilibrium between such atoms or molecules. Suitable examples include, but are not limited to covalent, electrostatic, hydrophobic, hydrophilic, hydrogen, and van der Waals bonding. The nature of such bonding relationships is known in the art and is described for instance in Mathews et al (1990) *Biochemistry,* Chapter 2, pgs 30-54.

As used herein, the terms "structure coordinates" and "structural coordinates" are interchangeable and mean mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule, for instance ErbB4K, in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal. Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for ErbB4 or a ErbB4K mutant that have a root mean square (RMS) deviation from ideal of no more than 1.5 Å, when superimposed using the polypeptide backbone atoms on the structure coordinates listed in Table 2, shall be considered identical, except that for the activation loop and nucleotide binding loop such deviation from ideal have a RMS of no more than 10 Å.

As used herein, the term "asymmetric unit" means part of a symmetric object from which the whole is built up by repeats. Thus, it is the smallest unit from which the object can be generated by the symmetry operations of its point group.

As used herein, the term "molecular replacement" means a method that involves generating a preliminary model of ErbB4 or ErbB4K mutant crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, (1985) in *Methods in Enzymology*, 115: 55-77). Using the structure coordinates of erbB4K and erbB4K in liganded form provided by this invention, molecular replacement can be used to determine the structure coordinates of a crystalline mutant or homologue of ErbB4K or of a different crystal form of ErbBK.

As used herein, the terms "β-sheet" and "beta sheet" are interchangeable and mean the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

As used herein, the terms "α-helix" and "alpha helix" are interchangeable and mean the conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a left-handed or right-handed direction. The substituent groups of the amino

acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turn of the helix, which extends about 0.56 nm along the long axis.

As used herein, the term "mutant" means a polypeptide which is obtained by replacing at least one amino acid residue in a native erbB4 or erbB4K polypeptide with a different amino acid residue and/or by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native erbB4 or erbB4K and which has substantially the same three-dimensional structure as the native erbB4 or erbB4K from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (RMS deviation) of less than or equal to about 1.5 Å, (10 Å for the activation loop and nucleotide binding loop) when superimposed with the atomic structure coordinates of the native erbB4 or erbB4K from which the mutant is derived when at least about 50% to 100% of the Cα atoms of the native erbB4 or erbB4K are included in the superposition. A mutant can have, but need not have, autophosphorylation activity.

As used herein, the term "space group" means a group or array of operations consistent with an infinitely extended regularly repeating pattern. It is the symmetry of a three-dimensional structure, or the arrangement of symmetry elements of a crystal. There are 230 space group symmetries possible; however, there are only 65 space group symmetries available for biological structures.

As used herein, the term "symmetry" means some spatial manipulation of an object resulting in an indistinguishable object. A symmetric object can, therefore, be superimposed on itself by some operation.

As used herein, the term "unit cell" means the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles α, β and γ define the angles between the vectors: angle α is the angle between vectors b and c; angle β is the angle between vectors a and c; and angle γ is the angle between vectors a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

As used herein, "monoclinic unit cell" means a unit cell wherein $a \neq b \neq c$ and $\alpha = \gamma = 90^{o}$ and $\beta \neq 90^{o}$. The vectors a, b and c describe the unit cell edges and the angles α, β, and γ describe the unit cell angles.

As used herein, "orthorhombic unit cell" means a unit cell wherein $a \neq b \neq c$; and $\alpha = \beta = \gamma = 90^{o}$. The vectors a, b and c describe the unit cell edges and the angles α, β, and γ describe the unit cell angles.

As used herein, the term "crystal lattice" means the array of points defined by the vertices of packed unit cells.

As used herein, the term "active site" means that site in the erbB4K domain where substrate peptide binding, ATP binding and catalysis occur. For erbB4, the active site comprises at least the activation loop and the nucleotide binding loop.

As used herein, the term "activation loop" refers to a loop in tyrosine kinase domains between the conserved AspPheGly sequence and the conserved AlaProGlu sequence that is believed to act as a regulatory loop.

As used herein the terms "nucleotide-binding loop" and "glycine-rich loop" are synonomous and mean a loop in an RTK which contains the protein kinase-conserved glycine-rich consensus sequence.

As used herein, the term "autophosphorylation site" means a residue or residues in erbB4K that is phosphorylated by a domain of erbB4 itself.

As used herein the term "juxtamembrane region" means that portion of erbB4K located between the transmembrane helix and the tyrosine kinase domain.

As used herein, the terms "kinase insert" and "kinase insert domain" are synonymous and mean an additional domain not found in non-receptor tyrosine kinases or serine/threonine kinases. It is found between helices αD and αE in the C-terminal domain of receptor tyrosine kinases and can vary greatly in sequence and length.

As used herein, the term "C-terminal tail" means that region of an RTK that extends beyond the final helix of the C-terminal domain of the RTK.

As used herein, the term "N-terminal domain" means that region of an RTK that has a defined structure and precedes in sequence the hinge region.

As used herein, the term "modulate" means an increase, decrease, or other alteration of any or all chemical and biological activities or properties of a wild-type or mutant erbB4 or erbB4K polypeptide.

Description of ErbB4K structure

The overall architecture of ErbB4K was analogous to structures reported previously for both serine/threonine and tyrosine protein kinases (Johnson et al, Cell, 85: 149-158; Cox et al, Curr. Opin. Struct. Biol., 4: 893-901). A C_α trace of ErbB4 is shown in Figure 2, where kinase secondary structural elements are labeled according to the convention originally given for cAPK (Knighton et al, Science, 253:407-413). ErbB4K folds into two domains, with catalysis occurring in a cleft between the two domains. Residues in the N-terminal domain are primarily responsible for ligating ATP, while residues in the C-terminal domain are involved in catalysis and substrate binding.

The N-terminal domain (residues 690-801) folds into a twisted β-sheet and one α-helix. The larger C-terminal domain (residues 802-999) contains eight α-helices (αD-αI) and a set of anti-parallel β-strands (β6/ β7). Strands 6 and 7 are positioned at the interdomain interface adjacent to the N-terminal β-sheet. Like other kinases, ErbB4K also contains functionally important loop regions: the glycine-rich nucleotide binding loop (residues 725-730), the catalytic loop (residues 841-848) and the activation loop (residues 861-890), which will be described in further detail below.

Activation loop

Protein kinases contain a large flexible loop, called the activation loop or A-loop, whose conformation is believed to regulate kinase activity. In many kinases, the conformation of the A-loop is controlled by the phosphorylation of specific residues within this region (Johnson et al). The

activation loop generally begins with a conserved AspPheGly sequence (ErbB4K 861) and ends at a conserved AlaProGlu (ErbB4K 890, AlaLeuGlu in ErbB4K) (Johnson et al). In structures of inactive kinases, portions of this loop are often disordered. In those structures where the A loop is ordered, it often blocks either the substrate or ATP binding sites (Mohammadi et al; Wybenga-Groot et al; Hubbard et al – 1997; Hubbard et al – 1994; McTigue et al; and Xu et al). Upon phosphorylation, the A-loop is repositioned to contact residues in the C-terminal domain (Hubbard et al – 1997). The activating phosphate can then interact with a cluster of basic residues, which includes a conserved arginine (ErbB4K R842), that precedes the catalytic aspartate (ErbB4K D843). The aspartyl residue of the AspPheGly motif ligates a Mg^{2+} ion, which, in turn contacts the β and γ phosphates of ATP.

In ErbB4K, the activation loop corresponds to residues 861-890 and contains a single tyrosine at position 875. In the ErbB4K structure presented, the A-loop is completely ordered and does not significantly block either the ATP or substrate binding sites. Unlike other A loops observed to date, the A loop in ErbB4 contains a short helix (helix A') immediately following the AspPheGly motif.

In ErbB4, Tyr875 is found in a similar position within the A-loop as tyrosines required for activation of other tyrosine kinases. The side chain of this residue in the ErbB4K crystal structure is pointing towards the interior of the protein rather than solvent and its OH forms a hydrogen bond to the backbone carbonyl of Cys891. It is not clear whether phosphorylation of this tyrosine in ErbB4 is required for full activity of the kinase.

Nucleotide binding loop

The nucleotide binding loop (NB loop) contains residues responsible for binding the triphosphate moiety of ATP in the correct position for catalysis

(Johnson etal and Cox et al). This glycine-rich loop is believed to be quite flexible and is often either disordered or has high b-factors in many unliganded kinase structures sites (Mohammadi et al; Wybenga-Groot et al; Hubbard et al – 1997; Hubbard et al – 1994; McTigue et al; and Xu et al). In ErbB4K, this loop is ordered and occupies a similar position to that seen in other kinase structures.

Catalytic loop

The catalytic loop of protein kinases lies between αE and β7 and contains an invariant aspartic acid (D843 in ErbB4) that serves as the catalytic base in the phosphotransfer reaction (Johnson et al). The sequence (HRDLAARN), as well as the backbone and side chain positions of this loop are similar to those in the unliganded EphB2, FGFR1, Tie2, IRK and VEGFR2 and in the ternary phosphorylated IRK complex structures sites (Mohammadi et al; Wybenga-Groot et al; Hubbard et al – 1997; Hubbard et al – 1994; and McTigue et al).

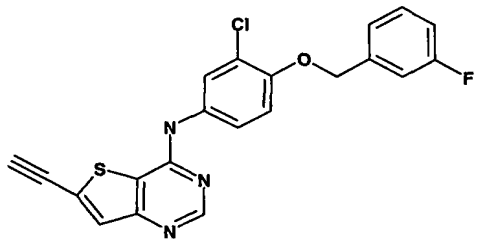
Inhibitor Binding Site

The ATP binding site can be broken down into several regions: hinge, adenine pocket, solvent interface, back pocket and sugar pocket. ATP is modeled into ErbB4 based on the activated IR structure. The hinge region runs from thr796 to pro800 and would be expected to form hydrogen bonds with the adenine base of ATP. The adenine pocket would be formed by the hinge residues on the side and ala749 and leu724 on top and leu850 on the bottom. The back pocket in ErbB4 is an elongated channel that can be divided by 2 regions defined by (1) val732, ala749, lys751, thr796, asp861, and thr860, and (2) met772, val781, leu783, leu794, thr796, and phe862. Typically, potential inhibitors bind in region (1) and do not reach back into region (2). A surface at the solvent interface formed by residues his801, gly802, cys803, glu806, and glu810 could form interactions with inhibitors.

The ribose or sugar pocket is defined by asn848, thr860, cys803, arg847, val732, and gly725.

Inhibitor/ErbB4K complex structure

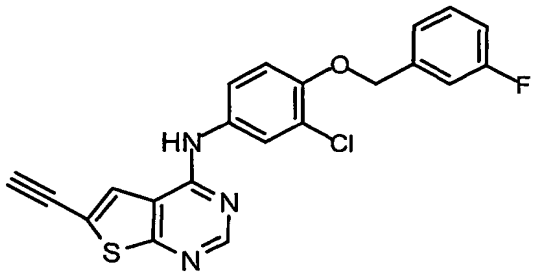
The structure of nonphosphorylated ErbB4 was solved in the presence of a thienopyrimidine inhibitor (formula Ia):



(Ia)

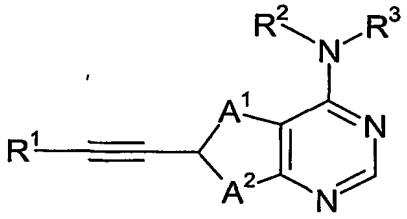
The inhibitor binds in the ATP binding site tunneling into the back of the pocket. The thienopyrimidine group, like the adenosine base of ATP, hydrogen bonds to the hinge region between the N and C-terminal domains (Figure 3). The inhibitor makes a single hydrogen bond to the protein. N1 of the inhibitor hydrogen bonds to the backbone NH of Met799. The thienopyrimidine ring is sandwiched from the top and bottom by the side chains of Ala749 and Leu850, respectively. The side chain of cys803 adds into the alkynyl group forming a cis double bond. The B and C rings of the inhibitor lie deep in the back of the ATP binding site. The B ring packs against the side chains of Val732, Ala749, Lys751, Thr796, and Thr860, while the C ring sits in a hydrophobic pocket formed by Met772, Val781, Leu783, Leu794, Thr796, and Phe862.

Co-crystal structures were also solved using the thienopyrimidine compound of formula (Ib):



(Ib)

Further compounds which may be co-crystallized with the ErbB4 kinase domain include compounds of formula (I):



(I)

wherein:

one of A^1 and A^2 is S and the other is CH;

R^1 is H or $-(CR^{11}R^{11})_n-R^5$;

R^2 is H or C_{1-6}alkyl;

R^3 is selected from the group consisting of aryl optionally substituted with one or more substituents selected from the group consisting of halo, alkynyl, $-CF_3$, $-(CH_2)_nOR^4$, $-(CH_2)_nSR^4$, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, $-(CH_2)_n$aryl and $-(CH_2)_nNR^9R^{10}$, and heteroaryl optionally substituted with one or more

substituents selected from the group consisting of halo, alkynyl, $-CF_3$, $-(CH_2)_nOR^4$, $-(CH_2)_nSR^4$, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, $-(CH_2)_n$aryl and $-(CH_2)_nNR^9R^{10}$;

R^4 is selected from the group consisting of H, C_{1-6}alkyl, $-(CH_2)_nNR^9R^{10}$, $-(CH_2)_n$heterocyclyl, $-(CH_2)_n$aryl in which aryl is optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, arylC_{1-6}alkenylene in which aryl is optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, heteroarylC_{1-6}alkenylene in which heteroaryl is optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, and $-(CH_2)_n$heteroaryl in which heteroaryl is optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$;

R^5 is selected from the group consisting of heterocyclyl, $-N(R^6)-C(O)-N(R^6)(R^7)$, $-N(R^6)-C(S)-N(R^6)(R^7)$, $-N(R^6)-C(O)-OR^7$, $-N(R^6)-C(O)-(CH_2)_n-R^7$, $-N(R^6)-SO_2R^6$, $-(CH_2)_nNR^6R^7$, $-(CH_2)_nOR^7$, $-(CH_2)_nSR^8$, $-(CH_2)_nS(O)R^8$, $-(CH_2)_nS(O)_2R^8$, $-OC(O)R^8$, $-OC(O)OR^8$, $-C(O)NR^6R^7$, heteroaryl optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, and aryl optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$;

R^6 and R^7 are independently selected from the group consisting of H, C_{1-6}alkyl, C_{3-8}cycloalkyl, heterocyclyl, $-(CH_2)_nNR^9R^{10}$, $-(CH_2)_nOR^9$, $-(CH_2)_nC(O)R^8$, $-C(O)_2R^8$, $-(CH_2)_nSR^8$, $-(CH_2)_nS(O)R^8$, $-(CH_2)_nS(O)_2R^8$, $-(CH_2)_nR^8$, $-(CH_2)_nCN$, aryl optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-(CH_2)_nOR^8$,

$-(CH_2)_n$heterocyclyl, $-(CH_2)_n$heteroaryl, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, and heteroaryl optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-(CH_2)_nOR^8$, $-(CH_2)_n$heterocyclyl, $-(CH_2)_n$heteroaryl, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, or R^6 and R^7, together with the atom to which they are attached, form a 3-8 membered ring;

R^8 is selected from the group consisting of C_{1-6}alkyl, C_{3-8}cycloalkyl, heterocyclylC_{1-6}alkylene, arylC_{1-6}alkylene wherein said aryl is optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, heteroarylC_{1-6}alkylene wherein said heteroaryl is optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, aryl optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$, and heteroaryl optionally substituted with one or more substituents selected from the group consisting of halo, $-CF_3$, C_{1-6}alkoxy, $-NO_2$, C_{1-6}alkyl, -CN, $-SO_2R^9$, and $-(CH_2)_nNR^9R^{10}$;

R^9 and R^{10} are independently selected from the group consisting of H, C_{1-6}alkyl, C_{3-8}cycloalkyl, and $-C(O)R^{11}$ or R^9 and R^{10}, together with the atom to which they are attached, form a 3-8 membered ring;

R^{11} is independently selected from the group consisting of H, C_{1-6}alkyl, and C_{3-8}cycloalkyl; and

n is 0-6.

Such thienopyrimidines are described in US Provisional Patent Application Ser. No. 60/342,207 filed December 19, 2001 which was filed December 13, 2002 as PCT Patent Application No. PCT/US02/39872 and

published as WO 03/053446 on July 3, 2003. Such applications are incorporated herein by reference to the extent they disclose and describe such thienopyrimidines as well as the making and use thereof.

As recited above, the present invention provides an ErbB4 kinase domain in liganded crystalline form. Such ErbB4 liganded kinase domain is described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2. SEQ ID NO: 1 is encoded by the DNA sequence of SEQ ID NO: 2. In another embodiment, is an ErbB4 liganded kinase domain described by the amino acid sequence encoded by the DNA sequence of SEQ ID NO: 2 and the structural coordinates of Table 2. In a further embodiment, is a substantially pure and isolated ErbB4 liganded kinase domain described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2. In another embodiment, is a substantially pure and isolated ErbB4 liganded kinase domain described by the amino acid sequence encoded by the DNA sequence of SEQ ID NO: 2 and the structural coordinates of Table 2.

In one embodiment the liganded ErbB4 kinase domain in crystalline form has lattice constants of a = 63.95 Å, b = 63.95 Å, c = 163.95 Å, α = 90°, β = 90°, and γ= 90°. In one embodiment, the liganded ErbB4 kinase domain in crystalline form has a space group of $P4_3$. In another embodiment, the liganded ErbB4 kinase in crystalline form has an entire NT region which is ordered. In still another embodiment, the liganded ErbB4 kinase in crystalline form has structural coordinates having a deviation from ideal with a RMS of no more than 1.5 Å except that the activation loop and/or a nucleotide binding loop have structural coordinates having a deviation from ideal with a RMS of no more than 10 Å. In a further embodiment, the liganded ErbB4 kinase in crystalline form has an activation loop and/or a nucleotide binding loop have structural coordinates having a deviation from ideal with a RMS of no more than 10 Å.

In another embodiment, there is provided an ErbB4 kinase domain/inhibitor complex which includes an ErbB4 liganded kinase domain described by the amino acid sequence of SEQ ID NO: 1 or 2 and the structural coordinates of Table 2 and a compound capable of at least one of the following interactions with the cFMS kinase domain:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket;

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket;

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket; and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface;

preferably

(i) one or more interactions with amino acid residues 796, 797, 798, 799, and 800;

(ii) one or more interactions with amino acid residues 724, 749, and 850;

(iii) one or more interactions with amino acid residues 848, 860, 803, 847, 732, and 725;

(iv) one or more interactions with amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862; and

(v) one or more interactions with residues 801, 802, 803, 806, and 810.

More preferred embodiments of interactions (i), (ii), (iii), (iv), and (v) are described following.

The amino acid region referred to in the interaction described in (i), which include amino acid residues 796 - 800, is typically referred to as the hinge region. In one embodiment, there are one or more kinase domain/compound bonding interactions with at least one of amino acid residues 796 to 800, preferably at least one of the bonding interactions is a hydrogen bonding interaction. In another embodiment, there are two or more bonding interactions with at least one of amino acid residues 796 to 800, preferably at least one of the bonding interactions is a hydrogen bonding interaction. In a further embodiment, there are three or more bonding interactions with at least one of amino acid residues 796 to 800, preferably at least one of the bonding interactions is a hydrogen bonding interaction. In a still further embodiment, there are four or more bonding interactions with at least one of amino acid residues 796 to 800, preferably at least one of the bonding interactions is a hydrogen bonding interaction.

In a preferred embodiment, there are one or more kinase domain/compound hydrogen bonding interactions with at least one of amino acid residues 796 to 800, alternatively two or more hydrogen bonding interactions with at least one of amino acid residues 796 to 800, in a further alternative embodiment three or more hydrogen bonding interactions with at least one of amino acid residues 796 to 800, and in a still further embodiment four or more bonding interactions with at least one of amino acid residues 796 to 800.

In a more preferred embodiment, there is a kinase domain/compound hydrogen bonding interaction with methionine 799, preferably one hydrogen bonding interaction with the backbone NH of methionine 799. Typically, this

hydrogen bond is at a distance of 2.5 to 3.5, preferably 2.6 to 3.3, more preferably 2.8 to 3.0 Å.

In another embodiment, there is a kinase domain/compound hydrogen bonding interaction with methionine 799 and there are one or more kinase domain/compound bonding interactions with at least one of amino acid residues 796 to 800. In another embodiment, there is a kinase domain/compound hydrogen bonding interaction with methionine 799 and there are two or more bonding interactions with at least one of amino acid residues 796 to 800. In a further embodiment, there is a kinase domain/compound hydrogen bonding interaction with methionine 799 and there are three or more bonding interactions with at least one of amino acid residues 796 to 800. Finally, in a still further embodiment, there is a kinase domain/compound hydrogen bonding interaction with methionine 799 and there are four or more bonding interactions with at least one of amino acid residues 796 to 800. Preferably, the one of the hydrogen bonding interactions with methionine 799 is with the backbone NH of methionine 799. Typically, this hydrogen bond is at a distance of 2.5 to 3.5, preferably 2.6 to 3.3, more preferably 2.8 to 3.0.

The amino acid region referred to in the interaction described in (ii), which includes amino acid residues 749, 724, and 850, is commonly termed the adenine pocket. In one embodiment, there are one or more kinase domain/compound interactions with at least one of amino acid residues 749, 724, and 850, preferably two or more interactions with at least two of amino acid residues 749, 724, and 850, more preferably three or more interactions with at least three of amino acid residues 749, 724, and 850, most preferably four or more bonding interactions with amino acid residues 749, 724, and 850.

In one embodiment, there is a kinase domain/compound hydrophobic interaction with alanine 749, preferably an interaction with the side chain of alanine 749. In another embodiment, there is a kinase domain/compound interaction with leucine 724. In a further embodiment, there is a kinase domain/compound interaction with leucine 850, preferably an interaction with the side chain of leucine 850. In a more preferred embodiment, there is one kinase domain/compound interaction with at least one of alanine 749, leucine 724, and leucine 850. In a most preferred embodiment, there are two kinase domain/compound bonding interactions: (i) an interaction with the side chain of alanine 749 and ii) an interaction with the side chain of leucine 850.

The amino acid region referred to in the interactions described in (iii) describe what is commonly termed the sugar (ribose) pocket and is defined by amino acid residues 848, 860, 803, 847, 732, and 725. In one embodiment, there are one or more kinase domain/compound interactions with at least one of amino acid residues 848, 860, 803, 847, 732, and 725, preferably two or more interactions with amino acid residues 848, 860, 803, 847, 732, and 725.

In one embodiment, there is a kinase domain/compound interaction with asparagine 848. In another embodiment, there is a kinase domain/compound interaction with threonine 860. In another embodiment, there is a kinase domain/compound interaction with cysteine 803, preferably a covalent interaction between cysteine 803 and the compound, more preferably a covalent interaction between cysteine 803 and the alkynyl group of the compound forming a cis double bond. In another embodiment, there is a kinase domain/compound interaction with arginine 847. In another embodiment, there is a kinase domain/compound interaction with valine 732. In another embodiment, there is a kinase domain/compound interaction with glycine 725.

The amino acid region referred to in the interactions in (iv) described what is commonly termed the back pocket, which is formed by residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862. In one embodiment, there are one or more kinase domain/compound interactions with at least one of amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862, preferably two or more interactions with at least two of amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862, more preferably three or more interactions with at least three of amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862, still more preferably four or more bonding interactions with at least four of amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862.

In one embodiment, there is a kinase domain/compound interaction with valine 732, preferably a hydrophobic interaction with valine 732. In another embodiment, there is a kinase domain/compound interaction with alanine 749, preferably a hydrophobic bonding interaction with alanine 749. In another embodiment, there is a kinase domain/compound interaction with lysine 751, preferably a hydrophobic interaction with lysine 751. In a further embodiment, there is a kinase domain/compound interaction with threonine 796, preferably a hydrophobic interaction with threonine 796. In another further embodiment, there is a kinase domain/compound hydrophobic interaction with aspartic acid 861, preferably a hydrophobic interaction with aspartic acid 861. In another embodiment, there is a kinase domain/compound interaction with threonine 860, preferably a hydrophobic interaction with threonine 860. In another embodiment, there is a kinase domain/compound interaction with methionine 772, preferably a hydrophobic interaction with methionine 772. In another embodiment, there is a kinase domain/compound interaction with valine 781, preferably a hydrophobic

interaction with valine 781. In another embodiment, there is a kinase domain/compound interaction with leucine 783, preferably a hydrophobic interaction with leucine 783. In another embodiment, there is a kinase domain/compound interaction with leucine 794, preferably a hydrophobic interaction with leucine 794. In another embodiment, there is a kinase domain/compound interaction with threonine 796, preferably a hydrophobic interaction with threonine 796. In another embodiment, there is a kinase domain/compound interaction with phenylalanine 862, preferably a hydrophobic interaction with phenylalanine 862.

The amino acid region referred to in the interactions in (v) describe what is commonly termed the solvent interface, which is formed by residues 801, 802, 803, 806, and 810. In one embodiment, there are one or more kinase domain/compound interactions with at least one of amino acid residues 801, 802, 803, 806, and 810, preferably two or more interactions with at least two of amino acid residues 801, 802, 803, 806, and 810, more preferably three or more interactions with at least two of amino acid residues 801, 802, 803, 806, and 810.

In one embodiment, there is a kinase domain/compound interaction with histidine 801. In another embodiment, there is a kinase domain/compound interaction with glycine 802. In one embodiment, there is a kinase domain/compound interaction with cysteine 803. In another embodiment, there is a kinase domain/compound interactions glutamic acid 806. In a further embodiment, there is a kinase domain/compound interaction with glutamic acid 810.

The method of ErbB4 inhibitor design of the present invention includes as a first step: generating a three dimensional computer model which represents a ErbB4 kinase domain in liganded form, said kinase domain being

described by the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2. Typically, such a computer model of SEQ ID NO: 1 and the structural coordinates of Table 2 is constructed utilizing a commercially available software program. Software programs for generating three-dimensional graphical representations of molecules or portions thereof from a set of structural coordinates are well known and used in the art. Suitable examples of such computer programs for viewing or otherwise manipulating protein structures include, but are not limited to, the following: Midas (University of California, San Francisco), MidasPlus (University of California, San Francisco),MOIL (Univeristy of Illinois), Yummie (Yale University), Sybyl (Tripos, Inc.), Insight/Discover (Biosym Technologies), MacroModel (Columbia University), Quanta (Molecular Simulations, Inc.), CNS (Molecular Simulations, Inc.), Cerius (Molucular Simulations, Inc.), Alchemy (Tripos, Inc.), LabVision (Tripos, Inc.), Rasmol (Glaxo Research and Development), Ribbon (University of Alabama), NAOMI (Oxford University), Explorer Eyechem (Silicon Graphics, Inc.), Univision (Cray Research), Molscript (Uppsala University), Chem-3D (Cambridge Scientific), Chain (Baylor College of Medicine), O (Uppsala University), GRASP (Columbia University), X-Plor (Molecular Simulations, Inc., Yale University), Spartan (Wavefunction, Inc.), Catalyst (Molecular Simulations, Inc.), Molcadd (Tripos, Inc.), VMD (University of Illinois/Beckman Institute), Sculpt (Interactive Simulations, Inc.), Procheck (Brookhaven National Laboratory), DGEOM (QCPE), RE_VIEW (Brunel University), Modeller (Birbeck College, University of London), Xmol (Minnesota Supercomputing Center), Protein Expert (Cambridge Scientific), HyperChem (Hypercube), MD Display (University of Washington), PKB (National Center for Biotechnology Information, NIH), ChemX (Chemical Design, Ltd.), Cameleon (Oxford Molecular,Inc.), and Iditis (Oxford Molecular, Inc.).

Once the three dimensional model of the ErbB4 kinase domain is established candidate inhibitor compounds may be evaluated utilizing the model and the selected software application. Initially, it is understood that the term "evaluate" includes within its scope, without limitation, de novo inhibitor molecular design, computer-aided optimization of known candidate inhibitors, as well as computer-based selection of candidate inhibitors. Various computational analysis methods are known in the art for the evaluation of potential binding interactions between a polypeptide binding pocket and a candidate inhibitor molecule. Such methods typically utilize at least one of the software packages recited above and are known in the art. Computational and other evaluation methods are described for instance in U.S. Patents 6,251,620 and 6,356,845, such patents being incorporated herein by reference to the extent that they disclose computational and other evaluation methods for drug design, selection and/or optimization.

Examples of protein-inhibitor interactions which are screened for include potential covalent, electrostatic, hydrophobic, hydrophilic, van der Waals, and hydrogen bonding between the ErbB4 kinase molecule and candidate inhibitors as well as favorable candidate inhibitor conformations within the ErbB4 kinase binding pocket.

In one embodiment, evaluation of compounds as potential ErbB4 inhibitors using said model comprises identifying compounds capable of at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(vi) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface;

preferably

(i) one or more interactions with amino acid residues 796, 797, 798, 799, and 800;

(iii) one or more interactions with amino acid residues 724, 749, and 850;

(iii) one or more interactions with amino acid residues 848, 860, 803, 847, 732, and 725;

(iv) one or more interactions with amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862; and

(v) one or more interactions with residues 801, 802, 803, 806, and 810.

Further preferred embodments of the interactions (i), (ii), (iii), (iv), and (v) are as described above.

If evaluation indicates that a compound shows promise as a candidate inhibitor the compounds are selected for further testing based on said evaluation. An inhibitor candidate is generally sought which can exist in a conformation, which appears to be structurally compatible with at least a part of the ErbB4 kinase domain binding pocket. Such conformation will be sterically and energetically compatible with the ErbB4 kinase domain. Typically, the above listed non-covalent or secondary bonding interactions will be important in the interaction of the candidate inhibitor and the ErbB4 kinase domain. In addition, other conformational factors include the overall three dimensional structure and orientation of the candidate inhibitor within the protein structure, especially the binding pocket as well as spacial and

energetic relationships of the various functional groups of the candidate inhibitor and ErbB4 kinase domain which have potential for interaction. The further testing done typically is to evaluate the inhibitory effect on the kinase activity of ErbB4 and may take the form of enzyme or cell based assays as well as other assays known in the art for measuring the inhibitory effect on the kinase activity of ErbB4.

The present invention also provides a method of inhibiting ErbB4 in a mammal, which includes administering to said mammal a therapeutically effective amount of a compound that can form a complex with a ErbB4 kinase domain thereby resulting in a ErbB4 kinase domain in liganded form. Also provided is a method of treating a disorder characterized by inappropriate ErbB4 activity in a mammal which includes administering to said mammal a therapeutically effective amount of a compound that can form a complex with a ErbB4 kinase domain thereby resulting in a ErbB4 kinase domain in liganded form.

Compounds useful in the treatment methods of the present invention include those having interactions (i), (ii), (iii), (iv), and (v) with the ErbB4 kinase domain. Such interactions are as described above.

The inappropriate ErbB4 activity referred to herein is any ErbB4 activity that deviates from the normal ErbB4 activity expected in a particular mammalian subject. Inappropriate ErbB4 activity may take the form of, for instance, an abnormal increase in activity, or an aberration in the timing and or control of ErbB4 activity. Such inappropriate activity may result then, for example, from overexpression or mutation of the protein kinase leading to inappropriate or uncontrolled activation. Furthermore, it is also understood that unwanted ErbB4 activity may reside in an abnormal source, such as a malignancy. That is, the level of ErbB4 activity does not have to be abnormal

to be considered inappropriate, rather the activity derives from an abnormal source.

While it is possible that, for use in therapy, therapeutically effective amounts of the compounds described in the present invention, as well as salts, solvates and physiologically functional derivatives thereof, may be administered as the raw chemical, it is possible to present the active ingredient as a pharmaceutical composition. Accordingly, the invention further provides pharmaceutical compositions, which include therapeutically effective amounts of the compound described herein and salts, solvates and physiological functional derivatives thereof, and one or more pharmaceutically acceptable carriers, diluents, or excipients. The compounds of the formula (I) and salts, solvates and physiological functional derivatives thereof, are as described above. The carrier(s), diluent(s) or excipient(s) must be acceptable in the sense of being compatible with the other ingredients of the formulation and not deleterious to the recipient thereof. In accordance with another aspect of the invention there is also provided a process for the preparation of a pharmaceutical formulation including admixing a compound of the present invention or salts, solvates and physiological functional derivatives thereof, with one or more pharmaceutically acceptable carriers, diluents or excipients.

Pharmaceutical formulations may be presented in unit dose forms containing a predetermined amount of active ingredient per unit dose. Such a unit may contain, for example, 0.5mg to 1g, preferably 1mg to 700mg, more preferably 5mg to 100mg of a compound of the present invention, depending on the condition being treated, the route of administration and the age, weight and condition of the patient, or pharmaceutical formulations may be presented in unit dose forms containing a predetermined amount of active ingredient per unit dose. Preferred unit dosage formulations are those containing a daily dose or sub-dose, as herein above recited, or an

appropriate fraction thereof, of an active ingredient. Furthermore, such pharmaceutical formulations may be prepared by any of the methods well known in the pharmacy art.

Pharmaceutical formulations may be adapted for administration by any appropriate route, for example by the oral (including buccal or sublingual), rectal, nasal, topical (including buccal, sublingual or transdermal), vaginal or parenteral (including subcutaneous, intramuscular, intravenous or intradermal) route. Such formulations may be prepared by any method known in the art of pharmacy, for example by bringing into association the active ingredient with the carrier(s) or excipient(s).

Pharmaceutical formulations adapted for oral administration may be presented as discrete units such as capsules or tablets; powders or granules; solutions or suspensions in aqueous or non-aqueous liquids; edible foams or whips; or oil-in-water liquid emulsions or water-in-oil liquid emulsions.

For instance, for oral administration in the form of a tablet or capsule, the active drug component can be combined with an oral, non-toxic pharmaceutically acceptable inert carrier such as ethanol, glycerol, water and the like. Powders are prepared by comminuting the compound to a suitable fine size and mixing with a similarly comminuted pharmaceutical carrier such as an edible carbohydrate, as, for example, starch or mannitol. Flavoring, preservative, dispersing and coloring agent can also be present.

Capsules are made by preparing a powder mixture, as described above, and filling formed gelatin sheaths. Glidants and lubricants such as colloidal silica, talc, magnesium stearate, calcium stearate or solid polyethylene glycol can be added to the powder mixture before the filling operation. A disintegrating or solubilizing agent such as agar-agar, calcium

carbonate or sodium carbonate can also be added to improve the availability of the medicament when the capsule is ingested.

Moreover, when desired or necessary, suitable binders, lubricants, disintegrating agents and coloring agents can also be incorporated into the mixture. Suitable binders include starch, gelatin, natural sugars such as glucose or beta-lactose, corn sweeteners, natural and synthetic gums such as acacia, tragacanth or sodium alginate, carboxymethylcellulose, polyethylene glycol, waxes and the like. Lubricants used in these dosage forms include sodium oleate, sodium stearate, magnesium stearate, sodium benzoate, sodium acetate, sodium chloride and the like. Disintegrators include, without limitation, starch, methyl cellulose, agar, bentonite, xanthan gum and the like. Tablets are formulated, for example, by preparing a powder mixture, granulating or slugging, adding a lubricant and disintegrant and pressing into tablets. A powder mixture is prepared by mixing the compound, suitably comminuted, with a diluent or base as described above, and optionally, with a binder such as carboxymethylcellulose, an aliginate, gelatin, or polyvinyl pyrrolidone, a solution retardant such as paraffin, a resorption accelerator such as a quaternary salt and/or an absorption agent such as bentonite, kaolin or dicalcium phosphate. The powder mixture can be granulated by wetting with a binder such as syrup, starch paste, acadia mucilage or solutions of cellulosic or polymeric materials and forcing through a screen. As an alternative to granulating, the powder mixture can be run through the tablet machine and the result is imperfectly formed slugs broken into granules. The granules can be lubricated to prevent sticking to the tablet forming dies by means of the addition of stearic acid, a stearate salt, talc or mineral oil. The lubricated mixture is then compressed into tablets. The compounds of the present invention can also be combined with a free flowing inert carrier and compressed into tablets directly without going through the granulating or slugging steps. A clear or opaque protective coating consisting

of a sealing coat of shellac, a coating of sugar or polymeric material and a polish coating of wax can be provided. Dyestuffs can be added to these coatings to distinguish different unit dosages.

Oral fluids such as solution, syrups and elixirs can be prepared in dosage unit form so that a given quantity contains a predetermined amount of the compound. Syrups can be prepared by dissolving the compound in a suitably flavored aqueous solution, while elixirs are prepared through the use of a non-toxic alcoholic vehicle. Suspensions can be formulated by dispersing the compound in a non-toxic vehicle. Solubilizers and emulsifiers such as ethoxylated isostearyl alcohols and polyoxy ethylene sorbitol ethers, preservatives, flavor additive such as peppermint oil or natural sweeteners or saccharin or other artificial sweeteners, and the like can also be added.

Where appropriate, dosage unit formulations for oral administration can be microencapsulated. The formulation can also be prepared to prolong or sustain the release as for example by coating or embedding particulate material in polymers, wax or the like.

The compounds of the present invention, and salts, solvates and physiological functional derivatives thereof, can also be administered in the form of liposome delivery systems, such as small unilamellar vesicles, large unilamellar vesicles and multilamellar vesicles. Liposomes can be formed from a variety of phospholipids, such as cholesterol, stearylamine or phosphatidylcholines.

The compounds of the present invention and salts, solvates and physiological functional derivatives thereof may also be delivered by the use of monoclonal antibodies as individual carriers to which the compound molecules are coupled. The compounds may also be coupled with soluble

polymers as targetable drug carriers. Such polymers can include polyvinylpyrrolidone, pyran copolymer, polyhydroxypropylmethacrylamide - phenol, polyhydroxyethylaspartamidephenol, or polyethyleneoxidepolylysine substituted with palmitoyl residues. Furthermore, the compounds may be coupled to a class of biodegradable polymers useful in achieving controlled release of a drug, for example, polylactic acid, polepsilon caprolactone, polyhydroxy butyric acid, polyorthoesters, polyacetals, polydihydropyrans, polycyanoacrylates and cross-linked or amphipathic block copolymers of hydrogels.

Pharmaceutical formulations adapted for transdermal administration may be presented as discrete patches intended to remain in intimate contact with the epidermis of the recipient for a prolonged period of time. For example, the active ingredient may be delivered from the patch by iontophoresis as generally described in Pharmaceutical Research, 3(6), 318 (1986).

Pharmaceutical formulations adapted for topical administration may be formulated as ointments, creams, suspensions, lotions, powders, solutions, pastes, gels, sprays, aerosols or oils.

For treatments of the eye or other external tissues, for example mouth and skin, the formulations are preferably applied as a topical ointment or cream. When formulated in an ointment, the active ingredient may be employed with either a paraffinic or a water-miscible ointment base. Alternatively, the active ingredient may be formulated in a cream with an oil-in-water cream base or a water-in-oil base.

Pharmaceutical formulations adapted for topical administrations to the eye include eye drops wherein the active ingredient is dissolved or suspended in a suitable carrier, especially an aqueous solvent.

Pharmaceutical formulations adapted for topical administration in the mouth include lozenges, pastilles and mouth washes.

Pharmaceutical formulations adapted for rectal administration may be presented as suppositories or as enemas.

Pharmaceutical formulations adapted for nasal administration wherein the carrier is a solid include a coarse powder having a particle size for example in the range 20 to 500 microns which is administered in the manner in which snuff is taken, i.e. by rapid inhalation through the nasal passage from a container of the powder held close up to the nose. Suitable formulations wherein the carrier is a liquid, for administration as a nasal spray or as nasal drops, include aqueous or oil solutions of the active ingredient.

Pharmaceutical formulations adapted for administration by inhalation include fine particle dusts or mists, which may be generated by means of various types of metered, dose pressurised aerosols, nebulizers or insufflators.

Pharmaceutical formulations adapted for vaginal administration may be presented as pessaries, tampons, creams, gels, pastes, foams or spray formulations.

Pharmaceutical formulations adapted for parenteral administration include aqueous and non-aqueous sterile injection solutions which may contain anti-oxidants, buffers, bacteriostats and solutes which render the

formulation isotonic with the blood of the intended recipient; and aqueous and non-aqueous sterile suspensions which may include suspending agents and thickening agents. The formulations may be presented in unit-dose or multi-dose containers, for example sealed ampoules and vials, and may be stored in a freeze-dried (lyophilized) condition requiring only the addition of the sterile liquid carrier, for example water for injections, immediately prior to use. Extemporaneous injection solutions and suspensions may be prepared from sterile powders, granules and tablets.

It should be understood that in addition to the ingredients particularly mentioned above, the formulations may include other agents conventional in the art having regard to the type of formulation in question, for example those suitable for oral administration may include flavouring agents.

A therapeutically effective amount of a compound of the present invention will depend upon a number of factors including, for example, the age and weight of the animal, the precise condition requiring treatment and its severity, the nature of the formulation, and the route of administration, and will ultimately be at the discretion of the attendant physician or veterinarian. However, an effective amount of a compound of the present invention for the treatment of neoplastic growth, for example colon or breast carcinoma, will generally be in the range of 0.1 to 100 mg/kg body weight of recipient (mammal) per day and more usually in the range of 1 to 10 mg/kg body weight per day. Thus, for a 70kg adult mammal, the actual amount per day would usually be from 70 to 700 mg and this amount may be given in a single dose per day or more usually in a number (such as two, three, four, five or six) of sub-doses per day such that the total daily dose is the same. An effective amount of a salt or solvate, or physiologically functional derivative thereof, may be determined as a proportion of the effective amount of the compound of the present invention *per se*. It is envisaged that similar

dosages would be appropriate for treatment of the other conditions referred to above.

EXAMPLES

As used herein the symbols and conventions used in these processes, schemes and examples are consistent with those used in the contemporary scientific literature, for example, the *Journal of the American Chemical Society* or the *Journal of Biological Chemistry.* Standard single-letter or three-letter abbreviations are generally used to designate amino acid residues, which are assumed to be in the L-configuration unless otherw8ise noted. Unless otherwise noted, all starting materials were obtained from commercial suppliers and used without further purification.

Structure determination

Modeling and limited proteolysis of the entire intracellular domain of ErbB4 were used to define a construct suitable for structural studies (residues 690-999). A 6x-His tag was added at the N-terminus to aid in the purification. The construct was expressed in baculovirus-infected insect cells and purified by standard chromatographic procedures. Crystallization screens were performed using nonphosphorylated protein complexed with an irreversible inhibitor (Figure 1). Crystals were obtained in the tetragonal space group $P4_3$ with two molecules in the asymmetric unit.

The structure was solved by molecular replacement using the structure of the FGFR1 as a search model [molecule 1 of PDB entry 1FGK]. The structure was refined to an R-factor of 21% at 2.5 Å resolution (Table 1). 8 residues at the N-terminus, 7 residues at the C-terminus and 6 residues within a surface exposed loop (residues 754-761) were disordered and could not be modeled. The structure of the two molecules in the asymmetric unit was essentially identical with a $C\alpha$ rmsd of 0.20 Å.

Certain embodiments of the present invention will now be illustrated by way of example only.

Materials and Methods

Construct generation

A combination of limited proteolysis and modeling was used to define the construct for structural studies. First, the cytoplasmic domain of ErbB4 (residues 690-1309) was ligated in frame behind a 6xHis tag (MKKGHHHHHHG) in a pFastBac1 vector (Invitrogen). The cloned sequence was identical to that reported in GENBANK (L07868).

Limited proteolysis was performed on purified protein from the 6xHis-EphB4_690-1309 construct to define a smaller catalytic domain (see below for more details). Proteolysis suggested that both the C-terminus could be truncated. Therefore, a second construct was generated corresponding to residues 690-999 fused to a 6x his tag (MKKGHHHHHHG). The His-tagged kinase domain was cloned by PCR from the pFastBac1-His-EphB4_690-1309 construct and ligated into a pFastBac1 vector (Invitrogen).

Both constructs were transfected into *Spodoptera frugiperda* (*sf-9*) cells, single plaques were isolated, and high titer stocks were generated. The proteins were expressed and purified as described below.

Limited proteolysis

Purified 6xHis-ErbB4_690-1309 was digested with a panel of 8 proteases in a 96 well plate. 5 ug of 6xHis-ErbB4 (5 uL at 1 mg/mL) was added to 5 uL of 10 mg/mL protease in 20 uL of reaction buffer (50 mM Tris-HCl, pH 8.0, 100 mM NaCl). Reactions were stopped at 0.75, 2, and 18 hours

with 10 uL of 4x SDS-PAGE sample buffer. All digests where analyzed by SDS-PAGE (NuPAGE Novex 10% Bis-Tris gel, MES running buffer). Bands of interest were electroblotted on PVDF membrane and subjected to Edman sequencing.

Proteases used	Source (Boehringer Mannheim unless otherwise noted)
1.) Trypsin	catalogue # 1418475
2.) Chymotrypsin	catalogue # 1418467
3.) Lys C	catalogue # 1047825
4.) Glu C	catalogue # 1047817
5.) Asp N	catalogue # 1054589
6.) Arg C	catalogue # 1370529
7.) Thermolysin	catalogue # 161586
8.) Subtilisin	catalogue # 572908 (Calbiochem)

Protein Fermentation/Purification

Fermentation: Large-scale (2L) virus preparations for fermentation were made by infecting *Sf-9* cells growing in Grace's Supplemented medium (GIBCO/Life Technologies) + 0.1% capluronic® F-68 (GIBCO/Life Technologies) + 10% FBS (HyClone Laboratories) at a multiplicity of infection (MOI) of 0.1 in 6L shake flasks at 27.5°C and 120 RPM. Viral supernatants were harvested at 72 hours post-infection via centrifugation at 2500 RPM for 20 minutes. Viral titers were determined via ELISA. A 36L stirred bioreactor (University Research Glassware) was outfitted with external overhead stirrer & water bath and internal dip tubes, heat-transfer coil, paddle-style impeller and dO_2 probe. The bioreactor was inoculated with *Trichoplusia ni* (*T. ni*) cells [kindly obtained from JRH BioSciences (Woodland, CA)] at ~0.5 X 10^6/mL. The culture was grown in Ex-Cell™ 405 insect cell medium (JRH BioSciences). Temperature was maintained at 27.5°C using an external water

bath and an internal temperature probe & heat-transfer coil. Agitation was maintained at 30 RPM using an external overhead drive and an internal paddle-type impeller. Dissolved oxygen was maintained at 50% via sparging under the control of an internal dO_2 probe. Cells were allowed to double overnight at the above parameters, and the culture was then infected at a density of ~ 1 X 10^6/mL at MOI = 1. The culture was monitored daily for pH, glucose, lactate and glutamine levels as well as cell count and viability via trypan blue exclusion. Infection was allowed to proceed at the above parameters, and cells were harvested at 48 hours post-infection using a Centritech® 100 continuous flow centrifuge (DuPont). Concentrated cells were subsequently centrifuged at 2000 RPM for 20 minutes and washed with protease inhibitor buffer [1X Dulbecco's PBS (GIBCO/Life Technologies), 1 mM EDTA (Sigma), 1 mM p-aminobenzamidine (Sigma), 1 μg/mL aprotinin (Boehringer Mannheim), 1μg/mL leupeptin (Boehringer Mannheim)]. Cells were centrifuged again at 2000 RPM for 20 minutes. The supernatant was decanted, and the cells were flash frozen in a dry ice/ethanol bath and stored at –80°C until further purification.

Purification:

All operations were carried out at 4°C. Insect cells were resuspended and thawed in buffer A (25 mM HEPES pH 7.5, 750 mM NaCl, 10% glycerol, 25 mM imidazole) supplemented with a protease inhibitor cocktail (Sigma), 1mM $MgCl_2$ and 5μg/ml of DNAse I and RNAse. The cells were lysed with a Polytron homogenizer (Brinkmann) and then centrifuged for 1 hour at 30,000 g (14,000 rpm) in a Sorvall SLA 1500 rotor. The pelleted material was discarded, and the supernatant was filtered through a 4.5μ filter (PALL Corp.). The lysate was directly loaded onto a Ni-Chelating Sepharose FF column (Amersham Pharmacia). Before sample loading, the column was equilibrated with 5 column volumes (CV's) of buffer A. After sample loading, the column was washed for 5 CV's with buffer A. The protein was eluted with a 20 CV

linear gradient from 50 to 500 mM imidazole in buffer A. Fractions containing ErbB4K protein were analyzed by polyacrylamide gel electrophoresis and pooled. The pool was diluted 8 fold in Buffer B (20 mM HEPES, 20 mM NaH_2PO_4, pH 6.8, 10% glycerol) and loaded onto Ceramic HA (Bio-Rad) column previously equilibrated in buffer B. Active ErbB4 flows through and does not bind. The flow-through fraction was brought to 0.6M $(NH_4)_2SO_4$ by addition of a 2.5M $(NH_4)_2SO_4$ stock solution and the sample applied to a Phenyl HIC column previously equilibrated in buffer E (20 mM Tris-HCl, pH 7.5, 0.6M $(NH_4)_2SO_4$). A reverse linear gradient to 100% buffer F (20 mM Tris-HCl, pH 7.5, 10% glycerol) was used to elute protein. Fractions containing pure ErbB4 were pooled, aliquoted and stored at -80°C.

Preparation of Inhibitor Candidate Compounds

As used herein the symbols and conventions used in these processes, schemes and examples are consistent with those used in the contemporary scientific literature, for example, the *Journal of the American Chemical Society* or the *Journal of Biological Chemistry*. Standard single-letter or three-letter abbreviations are generally used to designate amino acid residues, which are assumed to be in the L-configuration unless otherwise noted. Unless otherwise noted, all starting materials were obtained from commercial suppliers and used without further purification. Specifically, the following abbreviations may be used in the examples and throughout the specification:

g (grams);	mg (milligrams);
L (liters);	mL (milliliters);
µL (microliters);	psi (pounds per square inch);
M (molar);	mM (millimolar);
mol (moles);	mmol (millimoles);

All references to ether are to diethyl ether; brine refers to a saturated aqueous solution of NaCl. Unless otherwise indicated, all temperatures are

expressed in °C (degrees Centigrade). All reactions are conducted under an inert atmosphere at room temperature unless otherwise noted.

^{1}H NMR spectra were recorded on a Varian VXR-300, a Varian Unity-300, a Varian Unity-400 instrument, a Brucker AVANCE-400, or a General Electric QE-300. Chemical shifts are expressed in parts per million (ppm, δ units). Coupling constants are in units of hertz (Hz). Splitting patterns describe apparent multiplicities and are designated as s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), m (multiplet), br (broad).

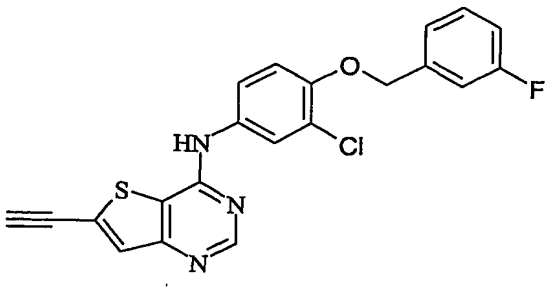
HPLC were recorded on a Gilson HPLC or Shimazu HPLC system by the following conditions. Column: 50 X 4.6mm (id) stainless steel packed with 5μm Phenomenex Luna C-18 ; Flow rate: 2.0 mL/min; Mobile phase: A phase = 50mM ammonium acetate (pH 7.4), B phase = acetonitrile, 0-0.5min (A: 100%, B: 0%), 0.5-3.0 min (A:100-0%, B:0-100%), 3.0-3.5min (A: 0%, B: 100%), 3.5-3.7 min (A: 0-100%, B: 100-0%), 3.7-4.5 min (A: 100%, B: 0%); Detection : UV 254nm; Injection volume: 3μL .

Low-resolution mass spectra (MS) were recorded on a JOEL JMS-AX505HA, JOEL SX-102, or a SCIEX-APIiii spectrometer; LC-MS were recorded on a micromass 2MD and Waters 2690; high resolution MS were obtained using a JOEL SX-102A spectrometer. All mass spectra were taken under electrospray ionization (ESI), chemical ionization (CI), electron impact (EI) or by fast atom bombardment (FAB) methods. Infrared (IR) spectra were obtained on a Nicolet 510 FT-IR spectrometer using a 1-mm NaCl cell. Most of the reactions were monitored by thin-layer chromatography on 0.25 mm E. Merck silica gel plates (60F-254), visualized with UV light, 5% ethanolic phosphomolybdic acid or p-anisaldehyde solution. Flash column chromatography was performed on silica gel (230-400 mesh, Merck).

Compounds of Formula I(a) and I(b) can be prepared according to the

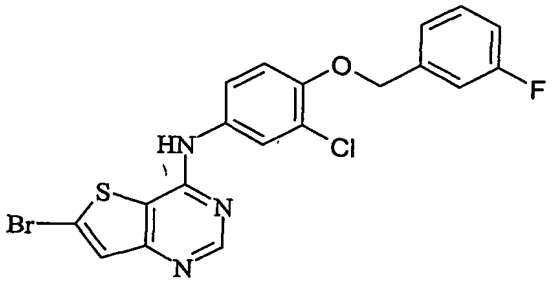
synthetic sequence detailed in the Examples section following.

Example 1
N-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-ethynylthieno[3,2-d]pyrimidin-4-amine



Step A

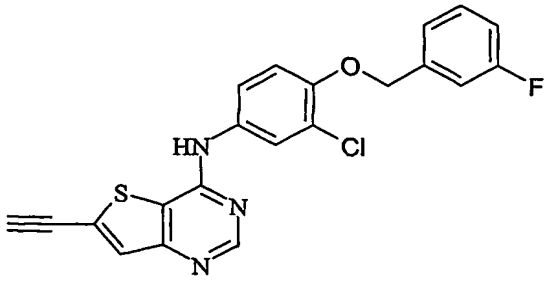
Preparation of 6-Bromo-N-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}thieno[3,2-d]pyrimidin-4-amine hydrochloride



6-Bromo-4-chlorothieno[3,2-*d*]pyrimidine (2) (1.05 g, 4 mmol) and 3-chloro-4-[(3-fluorobenzyl)oxy]aniline (986 mg, 3.9 mmol) were heated at 60 °C for 3 h in isopropanol (30 mL). The mixture was concentrated and the resulting material was triturated with ethyl ether and collected by suction filtration to yield the product (1.7 g) as a white solid.

Step B

Preparation of N-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-ethynylthieno[3,2-d]pyrimidin-4-amine



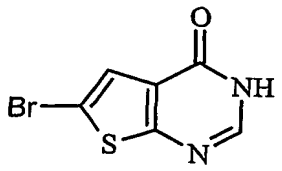
6-Bromo-*N*-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}thieno[3,2-*d*]pyrimidin-4-amine hydrochloride (1.0 g, 2.0 mmol) was combined with CuI (45 mg, 0.24 mmol), dichlorobis(triphenylphosphine)palladium(II) (57 mg, 0.08 mmol), THF (14 mL), triethylamine (0.74 mL, 5.3 mmol), and trimethylsilylacetylene (0.37 mL, 2.62 mmol). The mixture stirred at room temperature for 6 h, concentrated and purified by silica gel chromatography (eluting with 3:1 to 2:1 hexane/ethyl acetate). The resulting silyl acetylene intermediate (618 mg) was dissolved in THF (17 mL) and cooled to 0 °C. A 1.0 M solution of TBAF in THF (1.4 mL, 1.4 mmol) was added and the mixture was stirred 1 h. The reaction was partitioned between ethyl acetate and water, the organic layer was separated and dried (Na_2SO_4) filtered and concentrated. The resulting solid was purified by silica gel chromatography (eluting with 7:3 to 6:4 hexane/ethyl acetate) to give the title compound (400 mg) as an orange solid. ESI MS (positive ion): (M-H) 410.2

^{1}H NMR (300 MHz, DMSO) δ 5.03 (s, 1H), 5.25 (s, 2H), 7.14-7.21 (m, 1H), 7.23-7.22 (m, 3H), 7.43-7.50 (d, 1H), 7.61 (dd, J=8.9, 2.6Hz, 1H), 7.71 (s, 1H), 7.92 (d, J=2.5Hz, 1H), 8.59 (s, 1H), 9.78 (s, 1H).

Example 2
N-{3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-ethynylthieno[2,3-d]pyrimidin-4-amine

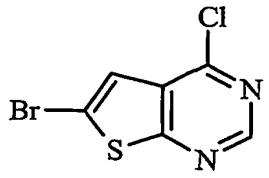
Step A

Preparation of 6-bromothieno[2 ,3-d]pyrimidin-4(3H)-one



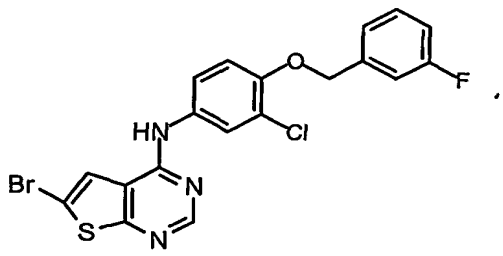
To a slurry of commercially available thieno[2,3-*d*]pyrimidin-4(3*H*)-one (1.5 g, 9.86 mmol) in glacial acetic acid (26 mL) was added dropwise bromine (1.0 mL, 20 mmol). The dark brown mixture was heated at 80 °C for 1.5 h. The mixture was allowed to cool to ambient temperature and was poured onto a mixture of saturated aqueous $NaHCO_3$ and ice. The resulting solid was collected by suction filtration, washed with water and dried in vacuo to afford 2.09 g of the title compound. ^1H NMR (400 MHz, DMSO-d_6) δ 7.54 (s, 1H), 8.13 (d, 2H, J = 3.7 Hz), 12.6 (bs, 1H).

Step B
Preparation of 6-Bromo-4-chlorothieno[2,3-d]pyrimidine



6-Bromothieno[2,3-d]pyrimidin-4(3H)-one (2.09 g, 9.05 mmol) was covered with phorphorous oxychloride (4.0 mL, 42.9 mmol) and the mixture was heated at 118-120 °C for 2 h. The mixture was allowed to cool to ambient temperature and was poured onto a mixture of saturated aqueous $NaHCO_3$ and ice. The resulting precipitate was collected by suction filtration and washed with water. The resulting solid was dried in vacuo to afford 2.07 g of the title compound. ^1H NMR (400 MHz, DMSO-d_6) δ 7.88 (s, 1H), 8.93 (s, 1H).

Step C
Preparation of 6-Bromo-N-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}thieno[2,3-d]pyrimidin-4-amine

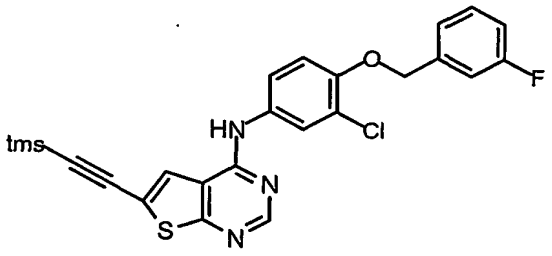


A mixture of 6-bromo-4-chlorothieno[2,3-d]pyrimidine (2.07 g, 8.29 mmol), 3-chloro-4-[(3-fluorobenzyl)oxy]aniline (2.09 g, 8.29 mmol),

triethylamine (2.31 mL, 16.57 mmol) and isopropanol (40 mL) was heated at 85 °C for 16 h. The mixture was allowed to cool to ambient temperature and concentrated to leave a brown residue. The mixture was triturated with ether to afford the title compound (3.34 g) as a tan solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.24 (s, 2H), 7.18 (m, 1H), 7.26 (d, 1H, J = 9.1 Hz), 7.32 (m, 1H), 7.64 (dd, 1H, J = 12.1, 2.7 Hz), 8.00 (d, 1H, J = 2.5 Hz), 8.02 (s, 1H), 8.48 (s, 1H), 9.63 (s, 1H).

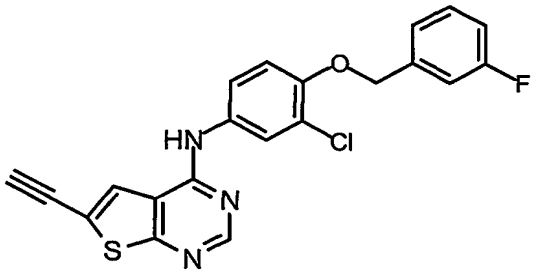
Step D

Preparation of N-{3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-[(trimethylsilyl)ethynyl]-4,4a-dihydrothieno[2,3-d]pyrimidin-4-amine



An N_2-flushed flask was charged with 6-bromo-*N*-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}thieno[2,3-*d*]pyrimidin-4-amine (1.0 g, 2.15 mmol), Cu(I)I (46 mg, 0.24 mmol), dichlorobis(triphenylphosphino)palladium(II) (57 mg, 0.081 mmol), anhydrous THF (13.5 mL), triethylamine (600 μL, 4.3 mmol) and trimethylsilyl acetylene (370 μL, 2.62 mmol) and the resulting mixture was heated at 40 °C for 5 h. The mixture was concentrated with a rotary evaporator and the residue was purified by flash silica gel chromatography (eluting with 5:1 hexanes/ethyl acetate) to afford 623.4 mg of the title compound as a yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 0.25 (s, 9H), 5.22 (s, 2H), 7.16 (dt, 1H, J = 8.9, 2.5 Hz), 7.24 (d, 1H, J = 9.0), 7.29 (m, 1H). 7.43 (m, 1H), 7.62 (dd, 1H, J = 8.9, 2.5 Hz), 8.01 (d, 1H, J = 2.8 Hz), 8.09 (s, 1H), 8.52 (s, 1H), 9.63 (s, 1H).

Step E
Preparation of N-{3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-ethynylthieno[2,3-d]pyrimidin-4-amine



To a 0 °C solution of *N*-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-[(trimethylsilyl)ethynyl]-4,4a-dihydrothieno[2,3-*d*]pyrimidin-4-amine (623.4 mg, 1.29 mmol) in anhydrous THF (17 mL) was added 1.0 M TBAF in THF (1.41 mL, 1.41 mmol). The mixture was stirred at 0 °C for 30 min, then partitioned between ethyl acetate and water. The organic layer was separated, dried over Na_2SO_4, filtered and concentrated to give a residue that was purified by silica gel chromatography (eluting with 5:1 hexanes/ethyl acetate) to give 519.3 mg of the title compound as a pale yellow solid, mp 197 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 4.89 (s, 1H), 5.27 (s, 2H), 7.21 (t, 1H, J = 9.2 Hz), 7.31 (d, 1H, J = 9.2 Hz), 7.34-7.36 (m, 1H). 7.45-7.50 (m, 1H), 7.67 (dd, 1H, J = 9.0, 2.4 Hz), 8.02 (d, 1H, J = 2.4 Hz), 8.10 (s, 1H), 8.56 (s, 1H), 9.75 (s, 1H). ms (MH)+ = 382.3.

ErbB4 Enzyme Assays:

Compounds of the present invention may be tested for ErbB-4 protein tyrosine kinase inhibitory activity in substrate phosphorylation assays using enzymes purified from a baculovirus expression system. Reagent production and assay methodology were conducted essentially as described (Brignola, P.S., et al, (2002) J. Biol. Chem. v. **277** in press).

The method measures the ability of the isolated enzyme to catalyse the transfer of the γ-phosphate from ATP onto tyrosine residues in a

biotinylated synthetic peptide (biotin-Ahx-RAHEEIYHFFFAKKK-amide). Reactions were performed in 96-well polystyrene round-bottom plates in a final volume of 45 μL. Reaction mixtures contained 50 mM MOPS (pH 7.5), 2 mM $MnCl_2$, 10 μM ATP, 0.125 μCi [γ-^{33}P] ATP per reaction, 2 μM peptide substrate, and 1mM dithiothreitol. Reactions were initiated by adding 1pmol (20nM) per reaction of the indicated enzyme. The reaction was allowed to proceed for 15 minutes, terminated and quantified using a scintillation proximity assay procedure as described in McDonald, O.B., Antonsson, B., Arkinstal, S., Marshall, C.J., and Wood, E.R. (1999) *Analytical Biochemistry*, **268**, 318-329.

Compounds under analysis were dissolved in Me_2SO to 0.5 mM and serially diluted 1 to 3 with Me_2SO through eleven columns of a 96 well plate. 1 μL of each concentration was transferred to the corresponding well of the assay plate. This creates a final compound concentration range from 0.00019 to 11.1 μM.

The data for dose responses were plotted as % Control calculated with the data reduction formula 100*(U1-C2)/(C1-C2) versus concentration of compound and fitted to the curve described by:

$y = ((Vmax * x) / (K + x))$

where Vmax is the upper asymptote and K is the IC_{50}. Typically, promising ErbB4 inhibitors will illicit a pIC50 > 7.0.

Crystallization and Data Collection

Crystals were obtained by the hanging drop vapor diffusion method. Protein (~4mg/ml in 20 mM HEPES pH 7.5, 300 mM NaCl, 5 mM DTT, 1mM CHAPS) was mixed with an equal volume of reservoir (50 mM cacodylate pH 6.5, 100 mM ammonium acetate, 10 mM Mg acetate, 30% PEG8000) and incubated at 22°C. Crystals belonged to the tetragonal space group $P4_3$ with

two molecules in the asymmetric unit and the following cell dimensions: a=63.95 Å, b=63.95 Å, c=163.39 Å, α=90°, β=90°, γ=90°.

Prior to data collection, glycerol and PEG400 was added to a final concentration of 25% and 5%, respectively, and the crystals were flash frozen in liquid N_2. Data was collected at beamline 17-BM on a MAR-CCD detector in the facilities of the Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT) at the Advanced Photon Source, Argonne National Laboratory. These facilities are supported by the companies of the Industrial Macromolecular Crystallography Association through a contract with Illinois Institute of Technology (IIT), executed through the IIT's Center for Synchrotron Radiation Research and Instrumentation. The data were processed using HKL2000.

Structure determination and refinement

The structure was solved by molecular replacement using CNX and FGFR1 as a search model (molecule 1 of PDB entry 1FGK). The search model contained FGFR1 residues 464-485, 491-500, 506-578, 592-647 and 651-761. Residues not conserved between FGFR1 and ErbB4 were truncated to alanine in the model. The correct solutions were the top two peaks in both the rotation and translation functions. Rigid body refinement gave an initial R-factor of 48%. Multiple rounds of model building and refinement were carried out with QUANTA and CNX. The overall structure was confirmed by a composite omit map calculated with CNX. Analysis of the structure with PROCHECK indicated that all main chain torsions fall within the allowed regions of the Ramachandran plot.

The results are depicted in Table 1 and 2 following.

(1) Amino Acid Sequence:

MKKGHHHHHHGLETELVEPLTPSGTAPNQAQLRILKETELKRVKVLGSGA
FGTVYKGIWVPEGETVKIPVAIKILNETTGPKANVEFMDEALIMASMDHP
HLVRLLGVCLSPTIQLVTQLMPHGCLLEYVHEHKDNIGSQLLLNWCVQIA
KGMMYLEERRLVHRDLAARNVLVKSPNHVKITDFGLARLLEGDEKEYNAD
GGKMPIKWMALECIHYRKFTHQSDVWSYGVTIWELMTFGGKPYDGIPTRE
IPDLLEKGERLPQPPICTIDVYMVMVKCWMIDADSRPKFKELAAEFSRMA
RDPQRYLVIQGDDRMKLPSPNDSKFFQNLLDEEDLEDMMDAEEYLVPQAF
NIPPPIYTSRARID (SEQ ID NO: 1)

DNA sequence 1: His-ErbB4amino acids 690-999 nucleotide sequence:

1	ATGAAAAAAG	GTCATCATCA	TCATCATCAT	GGTTTGGAAA	CAGAGTTGGT
51	GGAACCATTA	ACTCCCAGTG	GCACAGCACC	CAATCAAGCT	CAACTTCGTA
101	TTTTGAAAGA	AACTGAGCTG	AAGAGGGTAA	AAGTCCTTGG	CTCAGGTGCT
151	TTTGGAACGG	TTTATAAAGG	TATTTGGGTA	CCTGAAGGAG	AAACTGTGAA
201	GATTCCTGTG	GCTATTAAGA	TTCTTAATGA	GACAACTGGT	CCCAAGGCAA
251	ATGTGGAGTT	CATGGATGAA	GCTCTGATCA	TGGCAAGTAT	GGATCATCCA
301	CACCTAGTCC	GGTTGCTGGG	TGTGTGTCTG	AGCCCAACCA	TCCAGCTGGT
351	TACTCAACTT	ATGCCCCATG	GCTGCCTGTT	GGAGTATGTC	CACGAGCACA
401	AGGATAACAT	TGGATCACAA	CTGCTGCTTA	ACTGGTGTGT	CCAGATAGCT
451	AAGGGAATGA	TGTACCTGGA	AGAAAGACGA	CTCGTTCATC	GGGATTTGGC
501	AGCCCGTAAT	GTCTTAGTGA	AATCTCCAAA	CCATGTGAAA	ATCACAGATT
551	TTGGGCTAGC	CAGACTCTTG	GAAGGAGATG	AAAAAGAGTA	CAATGCTGAT
601	GGAGGAAAGA	TGCCAATTAA	ATGGATGGCT	CTGGAGTGTA	TACATTACAG
651	GAAATTCACC	CATCAGAGTG	ACGTTTGGAG	CTATGGAGTT	ACTATATGGG
701	AACTGATGAC	CTTTGGAGGA	AAACCCTATG	ATGGAATTCC	AACGCGAGAA
751	ATCCCTGATT	TATTAGAGAA	AGGAGAACGT	TTGCCTCAGC	CTCCCATCTG
801	CACTATTGAC	GTTTACATGG	TCATGGTCAA	ATGTTGGATG	ATTGATGCTG
851	ACAGTAGACC	TAAATTTAAG	GAACTGGCTG	CTGAGTTTTC	AAGGATGGCT
901	CGAGACCCTC	AAAGATACCT	AGTTATTCAG	GGTGATGATC	GTATGAAGCT
951	TCCCAGTCCA	AATTGA			

SEQ ID No : 2.

TABLE 1: DATA STATISTICS

Space group	$P4_3$	
Unit Cell a (Å)		63.95
Unit Cell b (Å)		63.95
Unit Cell c (Å)		163.39
Unit Cell $\alpha=\beta=\gamma$ (°)	90	
Mol/asu	2	
Resolution (Å)		2.5
R_{sym} (%)		8.8
Completeness (%)	91.9	
R_{factor} (%)	21	
R_{free} (%)		27
Rmsd from ideal		
Bond lengths (Å)	0.011	
Bond angles (°)		1.48

Table 2

erbB4(690-999) thienopyrimidine cocrystal
resolution: 500.0 - 2.5 A
sg= P4(3) a= 63.954 b= 63.954 c= 163.391 alpha= 90 beta= 90 gamma= 90
final r= 0.2130 free_r= 0.2762
rmsd bonds= 0.011188 rmsd angles= 1.48513
data completeness 91.9% Rmerge 8.8%
data collected on a marCCD at IMCA, -180C, processed with HKL2000, solved with CNX

ATOM	1	N	LEU A 698	-53.411	26.468	10.538	1.00	81.54
ATOM	2	CA	LEU A 698	-53.129	25.423	9.504	1.00	81.33
ATOM	3	C	LEU A 698	-53.233	26.015	8.103	1.00	81.09
ATOM	4	O	LEU A 698	-54.198	26.709	7.791	1.00	81.42
ATOM	5	CB	LEU A 698	-54.120	24.260	9.636	1.00	81.21
ATOM	6	CG	LEU A 698	-53.757	22.974	8.884	1.00	81.79
ATOM	7	CD1	LEU A 698	-52.552	22.311	9.555	1.00	81.75
ATOM	8	CD2	LEU A 698	-54.949	22.024	8.877	1.00	81.23
ATOM	9	N	THR A 699	-52.236	25.740	7.265	1.00	81.31
ATOM	10	CA	THR A 699	-52.210	26.243	5.890	1.00	82.23
ATOM	11	C	THR A 699	-51.171	25.519	5.018	1.00	82.37
ATOM	12	O	THR A 699	-50.003	25.905	4.971	1.00	82.32
ATOM	13	CB	THR A 699	-51.933	27.781	5.852	1.00	82.76
ATOM	14	OG1	THR A 699	-50.977	28.138	6.863	1.00	81.44
ATOM	15	CG2	THR A 699	-53.226	28.567	6.062	1.00	82.15
ATOM	16	N	PRO A 700	-51.593	24.452	4.315	1.00	82.54
ATOM	17	CA	PRO A 700	-50.743	23.642	3.435	1.00	82.57
ATOM	18	C	PRO A 700	-49.901	24.432	2.446	1.00	82.12
ATOM	19	O	PRO A 700	-50.175	25.596	2.159	1.00	82.75
ATOM	20	CB	PRO A 700	-51.747	22.741	2.724	1.00	82.43
ATOM	21	CG	PRO A 700	-52.758	22.504	3.777	1.00	82.66
ATOM	22	CD	PRO A 700	-52.958	23.898	4.353	1.00	83.18
ATOM	23	N	ALA A 701	-48.873	23.772	1.926	1.00	82.09
ATOM	24	CA	ALA A 701	-47.958	24.364	0.957	1.00	81.38
ATOM	25	C	ALA A 701	-47.697	23.318	-0.117	1.00	80.59
ATOM	26	O	ALA A 701	-47.769	22.118	0.149	1.00	81.14
ATOM	27	CB	ALA A 701	-46.646	24.755	1.643	1.00	81.49
ATOM	28	N	GLY A 702	-47.399	23.766	-1.328	1.00	79.29
ATOM	29	CA	GLY A 702	-47.139	22.814	-2.389	1.00	79.40
ATOM	30	C	GLY A 702	-46.042	21.833	-2.016	1.00	78.74
ATOM	31	O	GLY A 702	-46.226	20.612	-2.070	1.00	78.53
ATOM	32	N	THR A 703	-44.902	22.387	-1.615	1.00	77.41

ATOM	33	CA	THR A 703	-43.720	21.621	-1.238	1.00	75.67
ATOM	34	C	THR A 703	-43.960	20.300	-0.510	1.00	73.00
ATOM	35	O	THR A 703	-44.742	20.222	0.432	1.00	73.21
ATOM	36	CB	THR A 703	-42.780	22.481	-0.378	1.00	77.78
ATOM	37	OG1	THR A 703	-42.497	23.708	-1.065	1.00	78.99
ATOM	38	CG2	THR A 703	-41.473	21.740	-0.108	1.00	78.77
ATOM	39	N	ALA A 704	-43.259	19.264	-0.960	1.00	70.01
ATOM	40	CA	ALA A 704	-43.361	17.942	-0.366	1.00	66.51
ATOM	41	C	ALA A 704	-42.270	17.799	0.688	1.00	65.00
ATOM	42	O	ALA A 704	-41.318	18.588	0.737	1.00	63.04
ATOM	43	CB	ALA A 704	-43.201	16.872	-1.435	1.00	66.82
ATOM	44	N	PRO A 705	-42.395	16.788	1.552	1.00	62.77
ATOM	45	CA	PRO A 705	-41.399	16.577	2.597	1.00	61.58
ATOM	46	C	PRO A 705	-40.009	16.258	2.067	1.00	60.23
ATOM	47	O	PRO A 705	-39.843	15.521	1.095	1.00	61.36
ATOM	48	CB	PRO A 705	-41.993	15.430	3.410	1.00	61.65
ATOM	49	CG	PRO A 705	-42.736	14.656	2.391	1.00	63.07
ATOM	50	CD	PRO A 705	-43.418	15.730	1.581	1.00	63.22
ATOM	51	N	ASN A 706	-39.017	16.843	2.724	1.00	57.06
ATOM	52	CA	ASN A 706	-37.621	16.649	2.392	1.00	54.07
ATOM	53	C	ASN A 706	-37.112	15.494	3.264	1.00	53.97
ATOM	54	O	ASN A 706	-36.701	15.707	4.404	1.00	52.73
ATOM	55	CB	ASN A 706	-36.846	17.926	2.715	1.00	52.73
ATOM	56	CG	ASN A 706	-35.377	17.816	2.374	1.00	52.89
ATOM	57	OD1	ASN A 706	-34.883	16.732	2.070	1.00	51.75
ATOM	58	ND2	ASN A 706	-34.664	18.940	2.434	1.00	51.00
ATOM	59	N	GLN A 707	-37.137	14.274	2.740	1.00	51.97
ATOM	60	CA	GLN A 707	-36.679	13.147	3.536	1.00	53.28
ATOM	61	C	GLN A 707	-35.202	12.775	3.376	1.00	51.56
ATOM	62	O	GLN A 707	-34.813	11.628	3.611	1.00	50.32
ATOM	63	CB	GLN A 707	-37.563	11.925	3.280	1.00	52.48
ATOM	64	CG	GLN A 707	-38.988	12.125	3.736	1.00	57.13
ATOM	65	CD	GLN A 707	-39.850	10.906	3.491	1.00	60.12
ATOM	66	OE1	GLN A 707	-39.900	9.992	4.313	1.00	62.36
ATOM	67	NE2	GLN A 707	-40.523	10.876	2.338	1.00	60.48
ATOM	68	N	ALA A 708	-34.378	13.742	2.990	1.00	49.29
ATOM	69	CA	ALA A 708	-32.950	13.483	2.843	1.00	48.15
ATOM	70	C	ALA A 708	-32.400	13.031	4.202	1.00	48.57
ATOM	71	O	ALA A 708	-32.871	13.477	5.248	1.00	47.60
ATOM	72	CB	ALA A 708	-32.239	14.741	2.390	1.00	45.11
ATOM	73	N	GLN A 709	-31.416	12.138	4.187	1.00	49.32
ATOM	74	CA	GLN A 709	-30.824	11.662	5.430	1.00	49.62
ATOM	75	C	GLN A 709	-29.474	12.323	5.665	1.00	50.85
ATOM	76	O	GLN A 709	-28.692	12.528	4.736	1.00	52.52
ATOM	77	CB	GLN A 709	-30.627	10.145	5.388	1.00	48.60

```
ATOM    78  CG  GLN A 709     -31.897   9.345   5.182  1.00 47.70
ATOM    79  CD  GLN A 709     -32.848   9.427   6.353  1.00 47.21
ATOM    80  OE1 GLN A 709     -32.529   8.975   7.450  1.00 47.89
ATOM    81  NE2 GLN A 709     -34.027  10.004   6.126  1.00 44.74
ATOM    82  N   LEU A 710     -29.212  12.668   6.913  1.00 51.76
ATOM    83  CA  LEU A 710     -27.945  13.268   7.283  1.00 54.69
ATOM    84  C   LEU A 710     -27.458  12.404   8.424  1.00 55.52
ATOM    85  O   LEU A 710     -28.112  12.334   9.461  1.00 54.54
ATOM    86  CB  LEU A 710     -28.129  14.702   7.782  1.00 56.03
ATOM    87  CG  LEU A 710     -26.833  15.259   8.384  1.00 57.05
ATOM    88  CD1 LEU A 710     -25.863  15.544   7.264  1.00 56.49
ATOM    89  CD2 LEU A 710     -27.102  16.510   9.198  1.00 57.87
ATOM    90  N   ARG A 711     -26.321  11.742   8.247  1.00 56.82
ATOM    91  CA  ARG A 711     -25.821  10.877   9.302  1.00 58.00
ATOM    92  C   ARG A 711     -24.737  11.545  10.114  1.00 56.44
ATOM    93  O   ARG A 711     -23.756  12.036   9.577  1.00 55.70
ATOM    94  CB  ARG A 711     -25.327   9.556   8.710  1.00 60.89
ATOM    95  CG  ARG A 711     -26.351   8.925   7.763  1.00 67.44
ATOM    96  CD  ARG A 711     -25.971   7.525   7.317  1.00 71.94
ATOM    97  NE  ARG A 711     -26.098   6.561   8.406  1.00 76.65
ATOM    98  CZ  ARG A 711     -25.853   5.258   8.283  1.00 78.71
ATOM    99  NH1 ARG A 711     -25.465   4.760   7.111  1.00 78.46
ATOM   100  NH2 ARG A 711     -26.002   4.455   9.331  1.00 78.34
ATOM   101  N   ILE A 712     -24.946  11.584  11.422  1.00 57.82
ATOM   102  CA  ILE A 712     -23.988  12.181  12.342  1.00 59.70
ATOM   103  C   ILE A 712     -23.017  11.065  12.730  1.00 59.96
ATOM   104  O   ILE A 712     -23.401  10.089  13.363  1.00 59.83
ATOM   105  CB  ILE A 712     -24.727  12.748  13.562  1.00 59.41
ATOM   106  CG1 ILE A 712     -25.841  13.673  13.057  1.00 60.67
ATOM   107  CG2 ILE A 712     -23.760  13.512  14.469  1.00 57.78
ATOM   108  CD1 ILE A 712     -26.793  14.166  14.119  1.00 62.84
ATOM   109  N   LEU A 713     -21.761  11.215  12.328  1.00 60.81
ATOM   110  CA  LEU A 713     -20.753  10.191  12.566  1.00 62.74
ATOM   111  C   LEU A 713     -19.812  10.411  13.736  1.00 63.70
ATOM   112  O   LEU A 713     -19.297  11.512  13.939  1.00 63.91
ATOM   113  CB  LEU A 713     -19.907  10.007  11.307  1.00 62.56
ATOM   114  CG  LEU A 713     -20.661   9.698  10.016  1.00 62.99
ATOM   115  CD1 LEU A 713     -19.656   9.255   8.970  1.00 64.29
ATOM   116  CD2 LEU A 713     -21.714   8.620  10.254  1.00 62.63
ATOM   117  N   ALA A 714     -19.581   9.343  14.494  1.00 64.16
ATOM   118  CA  ALA A 714     -18.669   9.405  15.618  1.00 64.73
ATOM   119  C   ALA A 714     -17.294   9.443  14.978  1.00 65.80
ATOM   120  O   ALA A 714     -17.011   8.687  14.047  1.00 65.21
ATOM   121  CB  ALA A 714     -18.816   8.168  16.494  1.00 65.59
ATOM   122  N   GLU A 715     -16.461  10.352  15.470  1.00 67.13
```

```
ATOM   123  CA  GLU A 715     -15.092  10.556  15.000  1.00 68.35
ATOM   124  C   GLU A 715     -14.346   9.234  14.778  1.00 68.80
ATOM   125  O   GLU A 715     -13.419   9.145  13.965  1.00 67.36
ATOM   126  CB  GLU A 715     -14.370  11.404  16.046  1.00 70.35
ATOM   127  CG  GLU A 715     -12.937  11.784  15.762  1.00 74.38
ATOM   128  CD  GLU A 715     -12.337  12.568  16.925  1.00 76.58
ATOM   129  OE1 GLU A 715     -11.155  12.966  16.837  1.00 79.37
ATOM   130  OE2 GLU A 715     -13.051  12.785  17.932  1.00 75.16
ATOM   131  N   THR A 716     -14.779   8.211  15.509  1.00 68.91
ATOM   132  CA  THR A 716     -14.189   6.880  15.465  1.00 68.54
ATOM   133  C   THR A 716     -14.486   6.062  14.214  1.00 67.91
ATOM   134  O   THR A 716     -13.757   5.117  13.901  1.00 67.89
ATOM   135  CB  THR A 716     -14.643   6.049  16.675  1.00 69.38
ATOM   136  OG1 THR A 716     -14.187   4.700  16.521  1.00 72.15
ATOM   137  CG2 THR A 716     -16.163   6.049  16.782  1.00 69.99
ATOM   138  N   GLU A 717     -15.551   6.408  13.500  1.00 66.43
ATOM   139  CA  GLU A 717     -15.910   5.661  12.302  1.00 65.47
ATOM   140  C   GLU A 717     -15.111   6.104  11.085  1.00 64.70
ATOM   141  O   GLU A 717     -15.137   5.440  10.047  1.00 63.74
ATOM   142  CB  GLU A 717     -17.408   5.806  12.035  1.00 65.65
ATOM   143  CG  GLU A 717     -18.276   5.259  13.166  1.00 65.53
ATOM   144  CD  GLU A 717     -19.658   5.892  13.215  1.00 65.95
ATOM   145  OE1 GLU A 717     -20.471   5.662  12.291  1.00 62.49
ATOM   146  OE2 GLU A 717     -19.922   6.635  14.187  1.00 67.09
ATOM   147  N   LEU A 718     -14.382   7.211  11.223  1.00 64.90
ATOM   148  CA  LEU A 718     -13.591   7.752  10.119  1.00 65.63
ATOM   149  C   LEU A 718     -12.082   7.598  10.274  1.00 67.11
ATOM   150  O   LEU A 718     -11.521   7.846  11.345  1.00 66.91
ATOM   151  CB  LEU A 718     -13.909   9.236   9.917  1.00 64.23
ATOM   152  CG  LEU A 718     -15.353   9.609   9.575  1.00 64.11
ATOM   153  CD1 LEU A 718     -15.478  11.119   9.521  1.00 63.98
ATOM   154  CD2 LEU A 718     -15.757   8.988   8.251  1.00 62.29
ATOM   155  N   ALA A 719     -11.435   7.204   9.178  1.00 67.97
ATOM   156  CA  ALA A 719      -9.986   7.027   9.139  1.00 67.89
ATOM   157  C   ALA A 719      -9.394   7.806   7.968  1.00 67.48
ATOM   158  O   ALA A 719      -9.687   7.518   6.805  1.00 67.27
ATOM   159  CB  ALA A 719      -9.634   5.544   9.004  1.00 66.89
ATOM   160  N   ARG A 720      -8.572   8.801   8.284  1.00 67.63
ATOM   161  CA  ARG A 720      -7.918   9.605   7.264  1.00 67.22
ATOM   162  C   ARG A 720      -6.859   8.725   6.599  1.00 69.63
ATOM   163  O   ARG A 720      -6.763   7.534   6.890  1.00 70.38
ATOM   164  CB  ARG A 720      -7.230  10.810   7.901  1.00 65.71
ATOM   165  CG  ARG A 720      -8.103  11.668   8.793  1.00 65.13
ATOM   166  CD  ARG A 720      -7.881  13.135   8.465  1.00 65.92
ATOM   167  NE  ARG A 720      -8.268  14.063   9.529  1.00 67.39
```

```
ATOM    168  CZ  ARG A 720     -9.421  14.033  10.197  1.00 70.61
ATOM    169  NH1 ARG A 720    -10.342  13.103   9.939  1.00 70.23
ATOM    170  NH2 ARG A 720     -9.670  14.966  11.112  1.00 70.99
ATOM    171  N   VAL A 721     -6.060   9.315   5.716  1.00 71.34
ATOM    172  CA  VAL A 721     -4.988   8.599   5.018  1.00 71.66
ATOM    173  C   VAL A 721     -3.988   9.622   4.478  1.00 73.14
ATOM    174  O   VAL A 721     -3.027  10.001   5.157  1.00 73.20
ATOM    175  CB  VAL A 721     -5.533   7.764   3.833  1.00 70.82
ATOM    176  CG1 VAL A 721     -4.386   7.253   2.984  1.00 70.96
ATOM    177  CG2 VAL A 721     -6.344   6.592   4.347  1.00 70.37
ATOM    178  N   ALA A 722     -4.225  10.063   3.249  1.00 73.97
ATOM    179  CA  ALA A 722     -3.381  11.060   2.611  1.00 73.28
ATOM    180  C   ALA A 722     -4.262  12.283   2.405  1.00 72.83
ATOM    181  O   ALA A 722     -5.476  12.231   2.627  1.00 73.18
ATOM    182  CB  ALA A 722     -2.873  10.545   1.262  1.00 72.83
ATOM    183  N   VAL A 723     -3.640  13.381   1.996  1.00 71.49
ATOM    184  CA  VAL A 723     -4.356  14.615   1.728  1.00 68.53
ATOM    185  C   VAL A 723     -4.620  14.680   0.231  1.00 68.55
ATOM    186  O   VAL A 723     -3.765  14.319  -0.576  1.00 67.71
ATOM    187  CB  VAL A 723     -3.527  15.842   2.138  1.00 67.22
ATOM    188  CG1 VAL A 723     -4.174  17.111   1.605  1.00 66.63
ATOM    189  CG2 VAL A 723     -3.410  15.900   3.649  1.00 66.06
ATOM    190  N   LEU A 724     -5.815  15.120  -0.138  1.00 68.80
ATOM    191  CA  LEU A 724     -6.164  15.243  -1.542  1.00 68.52
ATOM    192  C   LEU A 724     -5.904  16.689  -1.969  1.00 69.72
ATOM    193  O   LEU A 724     -5.843  17.008  -3.156  1.00 71.11
ATOM    194  CB  LEU A 724     -7.630  14.859  -1.739  1.00 66.79
ATOM    195  CG  LEU A 724     -7.933  13.385  -1.456  1.00 65.65
ATOM    196  CD1 LEU A 724     -9.426  13.156  -1.423  1.00 65.45
ATOM    197  CD2 LEU A 724     -7.287  12.516  -2.526  1.00 66.07
ATOM    198  N   GLY A 725     -5.721  17.554  -0.979  1.00 70.85
ATOM    199  CA  GLY A 725     -5.467  18.954  -1.244  1.00 72.13
ATOM    200  C   GLY A 725     -6.098  19.804  -0.160  1.00 73.79
ATOM    201  O   GLY A 725     -6.806  19.290   0.707  1.00 73.67
ATOM    202  N   SER A 726     -5.842  21.106  -0.204  1.00 75.09
ATOM    203  CA  SER A 726     -6.400  22.022   0.780  1.00 76.38
ATOM    204  C   SER A 726     -6.234  23.459   0.316  1.00 76.97
ATOM    205  O   SER A 726     -5.127  23.899   0.005  1.00 77.58
ATOM    206  CB  SER A 726     -5.707  21.846   2.133  1.00 77.43
ATOM    207  OG  SER A 726     -4.369  22.314   2.090  1.00 77.62
ATOM    208  N   GLY A 727     -7.346  24.183   0.265  1.00 77.88
ATOM    209  CA  GLY A 727     -7.309  25.570  -0.151  1.00 77.49
ATOM    210  C   GLY A 727     -7.857  26.428   0.962  1.00 77.71
ATOM    211  O   GLY A 727     -7.950  25.984   2.107  1.00 76.78
ATOM    212  N   ALA A 728     -8.222  27.658   0.633  1.00 78.59
```

```
ATOM    213  CA  ALA A 728     -8.772  28.569   1.623  1.00 79.53
ATOM    214  C   ALA A 728    -10.094  28.003   2.130  1.00 80.29
ATOM    215  O   ALA A 728    -10.689  28.515   3.081  1.00 80.59
ATOM    216  CB  ALA A 728     -8.991  29.934   0.999  1.00 80.42
ATOM    217  N   PHE A 729    -10.533  26.924   1.495  1.00 80.52
ATOM    218  CA  PHE A 729    -11.789  26.283   1.845  1.00 80.77
ATOM    219  C   PHE A 729    -11.635  25.114   2.815  1.00 80.36
ATOM    220  O   PHE A 729    -12.611  24.430   3.122  1.00 81.24
ATOM    221  CB  PHE A 729    -12.480  25.821   0.563  1.00 81.06
ATOM    222  CG  PHE A 729    -12.521  26.879  -0.503  1.00 82.69
ATOM    223  CD1 PHE A 729    -11.372  27.197  -1.230  1.00 83.00
ATOM    224  CD2 PHE A 729    -13.690  27.601  -0.744  1.00 82.96
ATOM    225  CE1 PHE A 729    -11.385  28.222  -2.180  1.00 82.28
ATOM    226  CE2 PHE A 729    -13.712  28.625  -1.690  1.00 82.16
ATOM    227  CZ  PHE A 729    -12.555  28.936  -2.408  1.00 81.83
ATOM    228  N   GLY A 730    -10.417  24.895   3.307  1.00 78.97
ATOM    229  CA  GLY A 730    -10.176  23.800   4.234  1.00 75.86
ATOM    230  C   GLY A 730     -9.385  22.674   3.591  1.00 74.02
ATOM    231  O   GLY A 730     -9.022  22.756   2.418  1.00 74.18
ATOM    232  N   THR A 731     -9.124  21.613   4.347  1.00 71.57
ATOM    233  CA  THR A 731     -8.366  20.489   3.821  1.00 69.93
ATOM    234  C   THR A 731     -9.233  19.271   3.521  1.00 69.30
ATOM    235  O   THR A 731    -10.110  18.911   4.310  1.00 68.76
ATOM    236  CB  THR A 731     -7.255  20.078   4.795  1.00 70.50
ATOM    237  OG1 THR A 731     -6.360  21.180   4.985  1.00 69.99
ATOM    238  CG2 THR A 731     -6.479  18.893   4.244  1.00 69.46
ATOM    239  N   VAL A 732     -8.971  18.639   2.378  1.00 68.82
ATOM    240  CA  VAL A 732     -9.720  17.462   1.944  1.00 69.33
ATOM    241  C   VAL A 732     -8.852  16.202   1.933  1.00 70.00
ATOM    242  O   VAL A 732     -7.975  16.057   1.087  1.00 70.94
ATOM    243  CB  VAL A 732    -10.299  17.658   0.517  1.00 69.44
ATOM    244  CG1 VAL A 732    -11.149  16.457   0.143  1.00 69.31
ATOM    245  CG2 VAL A 732    -11.123  18.942   0.439  1.00 67.78
ATOM    246  N   TYR A 733     -9.112  15.291   2.867  1.00 70.94
ATOM    247  CA  TYR A 733     -8.361  14.040   2.980  1.00 70.76
ATOM    248  C   TYR A 733     -9.094  12.875   2.331  1.00 71.20
ATOM    249  O   TYR A 733    -10.322  12.862   2.263  1.00 70.51
ATOM    250  CB  TYR A 733     -8.164  13.661   4.449  1.00 73.12
ATOM    251  CG  TYR A 733     -7.466  14.679   5.318  1.00 75.05
ATOM    252  CD1 TYR A 733     -6.080  14.646   5.498  1.00 75.57
ATOM    253  CD2 TYR A 733     -8.193  15.665   5.984  1.00 75.38
ATOM    254  CE1 TYR A 733     -5.439  15.571   6.326  1.00 74.72
ATOM    255  CE2 TYR A 733     -7.564  16.594   6.809  1.00 75.15
ATOM    256  CZ  TYR A 733     -6.191  16.541   6.973  1.00 75.27
ATOM    257  OH  TYR A 733     -5.578  17.472   7.774  1.00 77.22
```

ATOM 258 N LYS A 734 -8.340 11.888 1.857 1.00 72.36
ATOM 259 CA LYS A 734 -8.955 10.688 1.294 1.00 72.08
ATOM 260 C LYS A 734 -9.168 9.821 2.534 1.00 71.34
ATOM 261 O LYS A 734 -8.445 9.984 3.524 1.00 69.91
ATOM 262 CB LYS A 734 -8.005 9.974 0.333 1.00 72.27
ATOM 263 CG LYS A 734 -8.519 8.605 -0.097 1.00 73.95
ATOM 264 CD LYS A 734 -7.471 7.804 -0.857 1.00 73.38
ATOM 265 CE LYS A 734 -7.982 6.400 -1.146 1.00 73.91
ATOM 266 NZ LYS A 734 -7.047 5.599 -1.976 1.00 72.92
ATOM 267 N GLY A 735 -10.139 8.913 2.512 1.00 70.61
ATOM 268 CA GLY A 735 -10.338 8.104 3.702 1.00 71.08
ATOM 269 C GLY A 735 -11.390 7.015 3.719 1.00 71.04
ATOM 270 O GLY A 735 -12.152 6.839 2.767 1.00 71.51
ATOM 271 N ILE A 736 -11.422 6.281 4.829 1.00 71.26
ATOM 272 CA ILE A 736 -12.368 5.188 5.005 1.00 72.22
ATOM 273 C ILE A 736 -13.364 5.496 6.107 1.00 72.21
ATOM 274 O ILE A 736 -13.003 6.023 7.161 1.00 71.05
ATOM 275 CB ILE A 736 -11.673 3.867 5.415 1.00 73.36
ATOM 276 CG1 ILE A 736 -10.379 3.663 4.621 1.00 74.33
ATOM 277 CG2 ILE A 736 -12.627 2.698 5.186 1.00 71.11
ATOM 278 CD1 ILE A 736 -9.552 2.470 5.102 1.00 75.22
ATOM 279 N TRP A 737 -14.618 5.146 5.858 1.00 72.87
ATOM 280 CA TRP A 737 -15.674 5.346 6.832 1.00 73.66
ATOM 281 C TRP A 737 -16.373 4.014 7.085 1.00 75.42
ATOM 282 O TRP A 737 -16.835 3.358 6.147 1.00 75.21
ATOM 283 CB TRP A 737 -16.681 6.383 6.328 1.00 71.21
ATOM 284 CG TRP A 737 -17.960 6.395 7.106 1.00 69.09
ATOM 285 CD1 TRP A 737 -18.096 6.373 8.466 1.00 68.36
ATOM 286 CD2 TRP A 737 -19.285 6.432 6.571 1.00 68.26
ATOM 287 NE1 TRP A 737 -19.426 6.391 8.810 1.00 67.91
ATOM 288 CE2 TRP A 737 -20.179 6.430 7.668 1.00 67.63
ATOM 289 CE3 TRP A 737 -19.806 6.470 5.271 1.00 67.83
ATOM 290 CZ2 TRP A 737 -21.565 6.463 7.506 1.00 67.13
ATOM 291 CZ3 TRP A 737 -21.189 6.503 5.107 1.00 68.96
ATOM 292 CH2 TRP A 737 -22.053 6.500 6.223 1.00 68.91
ATOM 293 N VAL A 738 -16.437 3.619 8.355 1.00 76.80
ATOM 294 CA VAL A 738 -17.085 2.374 8.746 1.00 78.00
ATOM 295 C VAL A 738 -18.328 2.714 9.563 1.00 79.76
ATOM 296 O VAL A 738 -18.226 3.062 10.736 1.00 80.23
ATOM 297 CB VAL A 738 -16.146 1.511 9.600 1.00 78.37
ATOM 298 CG1 VAL A 738 -16.738 0.125 9.772 1.00 77.43
ATOM 299 CG2 VAL A 738 -14.761 1.446 8.957 1.00 77.28
ATOM 300 N PRO A 739 -19.518 2.605 8.948 1.00 81.79
ATOM 301 CA PRO A 739 -20.837 2.887 9.531 1.00 83.53
ATOM 302 C PRO A 739 -21.013 2.624 11.025 1.00 85.81

```
ATOM   303  O   PRO A 739     -20.216   1.912  11.643  1.00 85.32
ATOM   304  CB  PRO A 739     -21.768   2.042   8.676  1.00 82.99
ATOM   305  CG  PRO A 739     -21.149   2.186   7.327  1.00 83.21
ATOM   306  CD  PRO A 739     -19.671   1.980   7.621  1.00 82.26
ATOM   307  N   ALA A 740     -22.076   3.207  11.585  1.00 87.67
ATOM   308  CA  ALA A 740     -22.407   3.091  13.008  1.00 89.23
ATOM   309  C   ALA A 740     -22.747   1.670  13.453  1.00 90.19
ATOM   310  O   ALA A 740     -23.730   1.456  14.170  1.00 90.44
ATOM   311  CB  ALA A 740     -23.571   4.031  13.345  1.00 88.58
ATOM   312  N   GLY A 741     -21.929   0.708  13.034  1.00 90.71
ATOM   313  CA  GLY A 741     -22.156  -0.680  13.396  1.00 91.14
ATOM   314  C   GLY A 741     -22.167  -1.612  12.199  1.00 91.59
ATOM   315  O   GLY A 741     -23.100  -2.396  12.025  1.00 91.52
ATOM   316  N   GLU A 742     -21.130  -1.528  11.369  1.00 91.74
ATOM   317  CA  GLU A 742     -21.033  -2.374  10.185  1.00 91.44
ATOM   318  C   GLU A 742     -19.579  -2.705   9.875  1.00 91.13
ATOM   319  O   GLU A 742     -18.667  -2.139  10.475  1.00 90.38
ATOM   320  CB  GLU A 742     -21.688  -1.680   8.986  1.00 91.24
ATOM   321  CG  GLU A 742     -23.106  -1.209   9.276  1.00 91.68
ATOM   322  CD  GLU A 742     -23.905  -0.905   8.027  1.00 92.00
ATOM   323  OE1 GLU A 742     -23.483  -0.040   7.232  1.00 91.88
ATOM   324  OE2 GLU A 742     -24.966  -1.538   7.844  1.00 91.68
ATOM   325  N   ALA A 743     -19.370  -3.625   8.936  1.00 91.28
ATOM   326  CA  ALA A 743     -18.024  -4.048   8.559  1.00 91.22
ATOM   327  C   ALA A 743     -17.472  -3.312   7.335  1.00 91.06
ATOM   328  O   ALA A 743     -16.276  -3.011   7.273  1.00 90.46
ATOM   329  CB  ALA A 743     -18.010  -5.559   8.307  1.00 90.34
ATOM   330  N   VAL A 744     -18.346  -3.025   6.371  1.00 90.80
ATOM   331  CA  VAL A 744     -17.950  -2.344   5.135  1.00 89.78
ATOM   332  C   VAL A 744     -17.025  -1.146   5.353  1.00 88.68
ATOM   333  O   VAL A 744     -17.191  -0.380   6.301  1.00 89.33
ATOM   334  CB  VAL A 744     -19.191  -1.867   4.323  1.00 89.22
ATOM   335  CG1 VAL A 744     -20.073  -3.053   3.983  1.00 89.59
ATOM   336  CG2 VAL A 744     -19.975  -0.831   5.111  1.00 88.82
ATOM   337  N   LYS A 745     -16.042  -0.999   4.469  1.00 86.57
ATOM   338  CA  LYS A 745     -15.098   0.111   4.542  1.00 84.05
ATOM   339  C   LYS A 745     -15.364   1.094   3.401  1.00 82.42
ATOM   340  O   LYS A 745     -14.580   1.174   2.460  1.00 81.96
ATOM   341  CB  LYS A 745     -13.655  -0.399   4.439  1.00 83.71
ATOM   342  CG  LYS A 745     -13.093  -1.055   5.696  1.00 82.67
ATOM   343  CD  LYS A 745     -11.580  -1.229   5.574  1.00 81.20
ATOM   344  CE  LYS A 745     -10.962  -1.742   6.864  1.00 81.60
ATOM   345  NZ  LYS A 745      -9.473  -1.807   6.792  1.00 80.27
ATOM   346  N   ILE A 746     -16.469   1.834   3.486  1.00 80.20
ATOM   347  CA  ILE A 746     -16.829   2.804   2.451  1.00 77.59
```

ATOM 348 C ILE A 746 -15.753 3.867 2.234 1.00 75.28
ATOM 349 O ILE A 746 -15.354 4.565 3.165 1.00 75.06
ATOM 350 CB ILE A 746 -18.153 3.521 2.784 1.00 78.03
ATOM 351 CG1 ILE A 746 -19.299 2.508 2.844 1.00 78.83
ATOM 352 CG2 ILE A 746 -18.451 4.568 1.726 1.00 79.05
ATOM 353 CD1 ILE A 746 -20.671 3.125 3.096 1.00 78.81
ATOM 354 N PRO A 747 -15.268 4.000 0.990 1.00 74.01
ATOM 355 CA PRO A 747 -14.235 4.985 0.654 1.00 71.83
ATOM 356 C PRO A 747 -14.866 6.370 0.601 1.00 70.14
ATOM 357 O PRO A 747 -15.882 6.574 -0.077 1.00 68.69
ATOM 358 CB PRO A 747 -13.753 4.510 -0.709 1.00 71.63
ATOM 359 CG PRO A 747 -15.018 4.016 -1.336 1.00 72.44
ATOM 360 CD PRO A 747 -15.673 3.237 -0.207 1.00 74.00
ATOM 361 N VAL A 748 -14.269 7.322 1.311 1.00 67.54
ATOM 362 CA VAL A 748 -14.820 8.669 1.346 1.00 65.96
ATOM 363 C VAL A 748 -13.797 9.791 1.302 1.00 64.98
ATOM 364 O VAL A 748 -12.584 9.565 1.370 1.00 63.82
ATOM 365 CB VAL A 748 -15.659 8.902 2.622 1.00 66.10
ATOM 366 CG1 VAL A 748 -16.839 7.953 2.666 1.00 65.30
ATOM 367 CG2 VAL A 748 -14.776 8.731 3.846 1.00 64.29
ATOM 368 N ALA A 749 -14.325 11.008 1.179 1.00 62.57
ATOM 369 CA ALA A 749 -13.525 12.221 1.172 1.00 61.68
ATOM 370 C ALA A 749 -14.004 12.942 2.411 1.00 61.42
ATOM 371 O ALA A 749 -15.204 13.026 2.656 1.00 62.73
ATOM 372 CB ALA A 749 -13.814 13.058 -0.060 1.00 60.54
ATOM 373 N ILE A 750 -13.070 13.432 3.212 1.00 60.76
ATOM 374 CA ILE A 750 -13.425 14.143 4.423 1.00 59.53
ATOM 375 C ILE A 750 -12.830 15.519 4.312 1.00 58.84
ATOM 376 O ILE A 750 -11.650 15.667 4.014 1.00 58.42
ATOM 377 CB ILE A 750 -12.855 13.456 5.671 1.00 59.88
ATOM 378 CG1 ILE A 750 -13.315 11.999 5.710 1.00 61.77
ATOM 379 CG2 ILE A 750 -13.312 14.193 6.917 1.00 59.44
ATOM 380 CD1 ILE A 750 -12.707 11.180 6.836 1.00 64.53
ATOM 381 N LYS A 751 -13.654 16.529 4.532 1.00 59.29
ATOM 382 CA LYS A 751 -13.188 17.897 4.458 1.00 60.16
ATOM 383 C LYS A 751 -13.373 18.529 5.814 1.00 61.42
ATOM 384 O LYS A 751 -14.406 18.347 6.463 1.00 60.51
ATOM 385 CB LYS A 751 -13.982 18.676 3.410 1.00 59.82
ATOM 386 CG LYS A 751 -13.519 20.109 3.247 1.00 59.02
ATOM 387 CD LYS A 751 -14.138 20.745 2.021 1.00 58.49
ATOM 388 CE LYS A 751 -13.435 22.035 1.690 1.00 57.20
ATOM 389 NZ LYS A 751 -13.915 22.606 0.411 1.00 58.47
ATOM 390 N ILE A 752 -12.365 19.271 6.242 1.00 63.64
ATOM 391 CA ILE A 752 -12.420 19.935 7.528 1.00 66.22
ATOM 392 C ILE A 752 -12.349 21.438 7.329 1.00 67.39

ATOM	393	O	ILE A 752	-11.394	21.945	6.749	1.00	67.55
ATOM	394	CB	ILE A 752	-11.256	19.473	8.422	1.00	66.68
ATOM	395	CG1	ILE A 752	-11.241	17.943	8.481	1.00	66.85
ATOM	396	CG2	ILE A 752	-11.404	20.065	9.818	1.00	67.28
ATOM	397	CD1	ILE A 752	-10.147	17.356	9.336	1.00	66.47
ATOM	398	N	ALA A 753	-13.372	22.146	7.799	1.00	70.53
ATOM	399	CA	ALA A 753	-13.419	23.602	7.673	1.00	74.64
ATOM	400	C	ALA A 753	-12.365	24.214	8.594	1.00	76.96
ATOM	401	O	ALA A 753	-11.877	23.534	9.500	1.00	77.82
ATOM	402	CB	ALA A 753	-14.806	24.110	8.038	1.00	73.77
ATOM	403	N	VAL A 754	-12.020	25.485	8.372	1.00	79.45
ATOM	404	CA	VAL A 754	-10.997	26.157	9.189	1.00	81.01
ATOM	405	CB	VAL A 754	-10.273	27.279	8.378	1.00	80.88
ATOM	406	CG1	VAL A 754	-8.977	27.694	9.096	1.00	78.71
ATOM	407	CG2	VAL A 754	-9.989	26.799	6.945	1.00	79.23
ATOM	408	C	VAL A 754	-11.541	26.769	10.494	1.00	82.00
ATOM	409	OT1	VAL A 754	-11.212	27.942	10.798	1.00	82.05
ATOM	410	OT2	VAL A 754	-12.277	26.057	11.216	1.00	82.11
ATOM	411	N	ALA A 761	-22.557	30.871	14.717	1.00	87.31
ATOM	412	CA	ALA A 761	-22.100	30.438	13.364	1.00	87.94
ATOM	413	C	ALA A 761	-22.469	28.982	13.071	1.00	88.76
ATOM	414	O	ALA A 761	-23.035	28.682	12.017	1.00	89.19
ATOM	415	CB	ALA A 761	-20.589	30.632	13.236	1.00	86.83
ATOM	416	N	ASN A 762	-22.147	28.080	13.995	1.00	88.98
ATOM	417	CA	ASN A 762	-22.459	26.666	13.812	1.00	89.06
ATOM	418	C	ASN A 762	-23.933	26.471	13.493	1.00	89.09
ATOM	419	O	ASN A 762	-24.339	25.428	12.975	1.00	89.26
ATOM	420	CB	ASN A 762	-22.083	25.865	15.060	1.00	89.85
ATOM	421	CG	ASN A 762	-20.608	25.519	15.102	1.00	90.47
ATOM	422	OD1	ASN A 762	-19.749	26.403	15.132	1.00	89.73
ATOM	423	ND2	ASN A 762	-20.306	24.225	15.098	1.00	90.01
ATOM	424	N	VAL A 763	-24.735	27.481	13.811	1.00	88.96
ATOM	425	CA	VAL A 763	-26.160	27.425	13.533	1.00	88.35
ATOM	426	C	VAL A 763	-26.274	27.447	12.020	1.00	88.39
ATOM	427	O	VAL A 763	-26.950	26.609	11.427	1.00	88.27
ATOM	428	CB	VAL A 763	-26.899	28.657	14.076	1.00	88.18
ATOM	429	CG1	VAL A 763	-28.380	28.348	14.200	1.00	87.36
ATOM	430	CG2	VAL A 763	-26.302	29.086	15.406	1.00	88.46
ATOM	431	N	GLU A 764	-25.598	28.420	11.408	1.00	87.88
ATOM	432	CA	GLU A 764	-25.599	28.574	9.956	1.00	86.88
ATOM	433	C	GLU A 764	-25.164	27.260	9.339	1.00	84.91
ATOM	434	O	GLU A 764	-25.826	26.724	8.448	1.00	85.31
ATOM	435	CB	GLU A 764	-24.609	29.654	9.507	1.00	88.52
ATOM	436	CG	GLU A 764	-24.708	30.982	10.231	1.00	90.41
ATOM	437	CD	GLU A 764	-23.821	32.047	9.600	1.00	91.24

ATOM 438 OE1 GLU A 764 -22.685 31.714 9.190 1.00 92.50
ATOM 439 OE2 GLU A 764 -24.254 33.218 9.523 1.00 91.08
ATOM 440 N PHE A 765 -24.037 26.751 9.823 1.00 81.83
ATOM 441 CA PHE A 765 -23.491 25.507 9.322 1.00 78.37
ATOM 442 C PHE A 765 -24.495 24.367 9.297 1.00 75.51
ATOM 443 O PHE A 765 -24.687 23.722 8.269 1.00 74.23
ATOM 444 CB PHE A 765 -22.280 25.080 10.141 1.00 79.06
ATOM 445 CG PHE A 765 -21.729 23.762 9.717 1.00 80.47
ATOM 446 CD1 PHE A 765 -22.371 22.577 10.079 1.00 81.96
ATOM 447 CD2 PHE A 765 -20.638 23.701 8.861 1.00 80.75
ATOM 448 CE1 PHE A 765 -21.945 21.353 9.586 1.00 81.90
ATOM 449 CE2 PHE A 765 -20.201 22.482 8.360 1.00 82.39
ATOM 450 CZ PHE A 765 -20.861 21.302 8.722 1.00 82.56
ATOM 451 N MET A 766 -25.117 24.092 10.433 1.00 72.71
ATOM 452 CA MET A 766 -26.083 23.014 10.472 1.00 70.93
ATOM 453 C MET A 766 -27.205 23.255 9.468 1.00 69.55
ATOM 454 O MET A 766 -27.946 22.338 9.120 1.00 70.42
ATOM 455 CB MET A 766 -26.638 22.849 11.887 1.00 71.33
ATOM 456 CG MET A 766 -25.603 22.336 12.873 1.00 71.61
ATOM 457 SD MET A 766 -24.622 20.959 12.199 1.00 74.04
ATOM 458 CE MET A 766 -25.720 19.631 12.348 1.00 69.51
ATOM 459 N ASP A 767 -27.331 24.489 8.995 1.00 66.54
ATOM 460 CA ASP A 767 -28.355 24.795 8.011 1.00 65.26
ATOM 461 C ASP A 767 -27.783 24.538 6.629 1.00 63.58
ATOM 462 O ASP A 767 -28.415 23.896 5.795 1.00 64.00
ATOM 463 CB ASP A 767 -28.807 26.249 8.131 1.00 67.20
ATOM 464 CG ASP A 767 -29.615 26.504 9.390 1.00 68.51
ATOM 465 OD1 ASP A 767 -30.624 25.794 9.594 1.00 68.20
ATOM 466 OD2 ASP A 767 -29.242 27.408 10.172 1.00 68.59
ATOM 467 N GLU A 768 -26.577 25.034 6.395 1.00 61.36
ATOM 468 CA GLU A 768 -25.917 24.841 5.118 1.00 60.21
ATOM 469 C GLU A 768 -25.744 23.350 4.846 1.00 58.77
ATOM 470 O GLU A 768 -25.834 22.908 3.704 1.00 58.90
ATOM 471 CB GLU A 768 -24.555 25.531 5.123 1.00 62.67
ATOM 472 CG GLU A 768 -23.938 25.709 3.745 1.00 68.86
ATOM 473 CD GLU A 768 -24.809 26.548 2.806 1.00 72.06
ATOM 474 OE1 GLU A 768 -24.346 26.888 1.696 1.00 75.67
ATOM 475 OE2 GLU A 768 -25.960 26.866 3.168 1.00 73.63
ATOM 476 N ALA A 769 -25.515 22.574 5.902 1.00 56.78
ATOM 477 CA ALA A 769 -25.329 21.134 5.764 1.00 53.94
ATOM 478 C ALA A 769 -26.602 20.437 5.328 1.00 53.30
ATOM 479 O ALA A 769 -26.547 19.423 4.626 1.00 55.21
ATOM 480 CB ALA A 769 -24.840 20.544 7.065 1.00 53.65
ATOM 481 N LEU A 770 -27.749 20.963 5.751 1.00 51.12
ATOM 482 CA LEU A 770 -29.029 20.373 5.370 1.00 50.39

```
ATOM   483  C   LEU A 770    -29.127  20.440   3.851  1.00 49.87
ATOM   484  O   LEU A 770    -29.584  19.502   3.194  1.00 48.92
ATOM   485  CB  LEU A 770    -30.206  21.136   6.019  1.00 49.49
ATOM   486  CG  LEU A 770    -31.615  20.629   5.648  1.00 50.99
ATOM   487  CD1 LEU A 770    -32.640  20.997   6.711  1.00 51.18
ATOM   488  CD2 LEU A 770    -32.026  21.204   4.295  1.00 48.88
ATOM   489  N   ILE A 771    -28.683  21.561   3.298  1.00 49.87
ATOM   490  CA  ILE A 771    -28.714  21.751   1.860  1.00 50.49
ATOM   491  C   ILE A 771    -27.728  20.805   1.175  1.00 50.51
ATOM   492  O   ILE A 771    -28.092  20.059   0.271  1.00 51.88
ATOM   493  CB  ILE A 771    -28.352  23.196   1.491  1.00 49.76
ATOM   494  CG1 ILE A 771    -29.258  24.175   2.249  1.00 51.25
ATOM   495  CG2 ILE A 771    -28.509  23.394  -0.006  1.00 48.11
ATOM   496  CD1 ILE A 771    -30.729  24.104   1.846  1.00 52.39
ATOM   497  N   MET A 772    -26.479  20.830   1.616  1.00 49.68
ATOM   498  CA  MET A 772    -25.469  19.976   1.023  1.00 49.48
ATOM   499  C   MET A 772    -25.925  18.544   1.041  1.00 49.90
ATOM   500  O   MET A 772    -25.504  17.748   0.216  1.00 53.68
ATOM   501  CB  MET A 772    -24.152  20.078   1.784  1.00 50.02
ATOM   502  CG  MET A 772    -23.670  21.485   1.974  1.00 50.14
ATOM   503  SD  MET A 772    -22.079  21.532   2.743  1.00 51.82
ATOM   504  CE  MET A 772    -21.416  23.034   1.966  1.00 54.26
ATOM   505  N   ALA A 773    -26.797  18.210   1.975  1.00 49.25
ATOM   506  CA  ALA A 773    -27.265  16.841   2.078  1.00 49.85
ATOM   507  C   ALA A 773    -28.569  16.559   1.339  1.00 49.63
ATOM   508  O   ALA A 773    -28.963  15.405   1.189  1.00 49.98
ATOM   509  CB  ALA A 773    -27.403  16.467   3.554  1.00 50.21
ATOM   510  N   SER A 774    -29.243  17.597   0.867  1.00 50.09
ATOM   511  CA  SER A 774    -30.507  17.385   0.172  1.00 51.17
ATOM   512  C   SER A 774    -30.366  17.304  -1.333  1.00 50.49
ATOM   513  O   SER A 774    -31.325  16.996  -2.027  1.00 53.51
ATOM   514  CB  SER A 774    -31.503  18.496   0.514  1.00 50.00
ATOM   515  OG  SER A 774    -31.733  18.568   1.903  1.00 53.58
ATOM   516  N   MET A 775    -29.181  17.578  -1.850  1.00 51.19
ATOM   517  CA  MET A 775    -28.991  17.536  -3.296  1.00 51.57
ATOM   518  C   MET A 775    -29.005  16.115  -3.879  1.00 50.46
ATOM   519  O   MET A 775    -28.128  15.298  -3.603  1.00 49.82
ATOM   520  CB  MET A 775    -27.701  18.277  -3.657  1.00 52.20
ATOM   521  CG  MET A 775    -27.711  19.720  -3.185  1.00 52.73
ATOM   522  SD  MET A 775    -29.349  20.470  -3.403  1.00 58.26
ATOM   523  CE  MET A 775    -29.044  21.567  -4.684  1.00 55.94
ATOM   524  N   ASP A 776    -30.022  15.836  -4.688  1.00 49.69
ATOM   525  CA  ASP A 776    -30.190  14.532  -5.309  1.00 47.92
ATOM   526  C   ASP A 776    -30.278  14.653  -6.819  1.00 46.24
ATOM   527  O   ASP A 776    -31.354  14.609  -7.411  1.00 43.09
```

```
ATOM    528  CB  ASP A 776     -31.442  13.853  -4.762  1.00 51.21
ATOM    529  CG  ASP A 776     -31.736  12.519  -5.434  1.00 54.67
ATOM    530  OD1 ASP A 776     -30.795  11.880  -5.970  1.00 54.64
ATOM    531  OD2 ASP A 776     -32.919  12.105  -5.407  1.00 56.04
ATOM    532  N   HIS A 777     -29.110  14.797  -7.428  1.00 45.15
ATOM    533  CA  HIS A 777     -28.977  14.929  -8.862  1.00 43.19
ATOM    534  C   HIS A 777     -27.687  14.220  -9.231  1.00 44.58
ATOM    535  O   HIS A 777     -26.690  14.324  -8.524  1.00 43.08
ATOM    536  CB  HIS A 777     -28.899  16.401  -9.239  1.00 41.16
ATOM    537  CG  HIS A 777     -28.776  16.641 -10.705  1.00 42.58
ATOM    538  ND1 HIS A 777     -27.601  16.439 -11.397  1.00 42.84
ATOM    539  CD2 HIS A 777     -29.684  17.063 -11.616  1.00 40.33
ATOM    540  CE1 HIS A 777     -27.791  16.728 -12.672  1.00 42.28
ATOM    541  NE2 HIS A 777     -29.047  17.109 -12.830  1.00 41.77
ATOM    542  N   PRO A 778     -27.690  13.484 -10.350  1.00 46.58
ATOM    543  CA  PRO A 778     -26.485  12.763 -10.768  1.00 47.00
ATOM    544  C   PRO A 778     -25.241  13.622 -10.969  1.00 47.70
ATOM    545  O   PRO A 778     -24.113  13.150 -10.775  1.00 48.99
ATOM    546  CB  PRO A 778     -26.930  12.047 -12.046  1.00 45.89
ATOM    547  CG  PRO A 778     -28.008  12.925 -12.575  1.00 45.82
ATOM    548  CD  PRO A 778     -28.773  13.323 -11.338  1.00 45.42
ATOM    549  N   HIS A 779     -25.415  14.890 -11.318  1.00 46.96
ATOM    550  CA  HIS A 779     -24.231  15.701 -11.533  1.00 46.65
ATOM    551  C   HIS A 779     -23.869  16.697 -10.426  1.00 46.00
ATOM    552  O   HIS A 779     -23.195  17.709 -10.640  1.00 43.82
ATOM    553  CB  HIS A 779     -24.318  16.330 -12.922  1.00 45.35
ATOM    554  CG  HIS A 779     -24.475  15.309 -14.009  1.00 46.09
ATOM    555  ND1 HIS A 779     -23.614  14.242 -14.153  1.00 45.56
ATOM    556  CD2 HIS A 779     -25.423  15.156 -14.966  1.00 46.11
ATOM    557  CE1 HIS A 779     -24.025  13.476 -15.148  1.00 44.45
ATOM    558  NE2 HIS A 779     -25.121  14.008 -15.658  1.00 43.34
ATOM    559  N   LEU A 780     -24.307  16.364  -9.222  1.00 45.67
ATOM    560  CA  LEU A 780     -23.985  17.141  -8.038  1.00 48.21
ATOM    561  C   LEU A 780     -23.651  16.086  -6.994  1.00 48.90
ATOM    562  O   LEU A 780     -24.192  14.979  -7.029  1.00 48.98
ATOM    563  CB  LEU A 780     -25.176  17.986  -7.572  1.00 48.42
ATOM    564  CG  LEU A 780     -25.561  19.240  -8.367  1.00 49.03
ATOM    565  CD1 LEU A 780     -26.749  19.886  -7.683  1.00 49.91
ATOM    566  CD2 LEU A 780     -24.408  20.229  -8.432  1.00 47.36
ATOM    567  N   VAL A 781     -22.746  16.398  -6.081  1.00 49.42
ATOM    568  CA  VAL A 781     -22.413  15.420  -5.060  1.00 51.41
ATOM    569  C   VAL A 781     -23.365  15.572  -3.882  1.00 53.85
ATOM    570  O   VAL A 781     -24.077  16.572  -3.762  1.00 53.60
ATOM    571  CB  VAL A 781     -20.969  15.592  -4.564  1.00 49.34
ATOM    572  CG1 VAL A 781     -19.998  15.434  -5.730  1.00 48.15
```

ATOM 573 CG2 VAL A 781 -20.809 16.942 -3.910 1.00 48.13
ATOM 574 N ARG A 782 -23.386 14.565 -3.018 1.00 57.31
ATOM 575 CA ARG A 782 -24.238 14.593 -1.834 1.00 58.51
ATOM 576 C ARG A 782 -23.429 14.365 -0.560 1.00 57.98
ATOM 577 O ARG A 782 -22.467 13.589 -0.537 1.00 58.11
ATOM 578 CB ARG A 782 -25.343 13.539 -1.943 1.00 59.06
ATOM 579 CG ARG A 782 -26.213 13.466 -0.718 1.00 64.02
ATOM 580 CD ARG A 782 -27.508 12.723 -0.986 1.00 69.63
ATOM 581 NE ARG A 782 -28.200 12.383 0.259 1.00 74.15
ATOM 582 CZ ARG A 782 -29.459 11.955 0.325 1.00 77.34
ATOM 583 NH1 ARG A 782 -30.173 11.821 -0.793 1.00 76.96
ATOM 584 NH2 ARG A 782 -29.999 11.642 1.504 1.00 76.96
ATOM 585 N LEU A 783 -23.817 15.063 0.497 1.00 57.15
ATOM 586 CA LEU A 783 -23.146 14.930 1.776 1.00 57.64
ATOM 587 C LEU A 783 -23.644 13.666 2.470 1.00 57.90
ATOM 588 O LEU A 783 -24.824 13.568 2.811 1.00 58.39
ATOM 589 CB LEU A 783 -23.454 16.147 2.649 1.00 56.99
ATOM 590 CG LEU A 783 -22.693 16.228 3.970 1.00 55.50
ATOM 591 CD1 LEU A 783 -21.204 16.354 3.679 1.00 54.23
ATOM 592 CD2 LEU A 783 -23.189 17.409 4.771 1.00 53.18
ATOM 593 N LEU A 784 -22.755 12.698 2.671 1.00 57.71
ATOM 594 CA LEU A 784 -23.137 11.456 3.341 1.00 57.94
ATOM 595 C LEU A 784 -23.412 11.744 4.809 1.00 57.07
ATOM 596 O LEU A 784 -24.453 11.360 5.353 1.00 57.68
ATOM 597 CB LEU A 784 -22.020 10.416 3.249 1.00 58.52
ATOM 598 CG LEU A 784 -21.758 9.742 1.905 1.00 61.56
ATOM 599 CD1 LEU A 784 -20.493 8.905 2.013 1.00 62.06
ATOM 600 CD2 LEU A 784 -22.950 8.881 1.499 1.00 60.90
ATOM 601 N GLY A 785 -22.472 12.433 5.446 1.00 55.42
ATOM 602 CA GLY A 785 -22.635 12.742 6.848 1.00 54.66
ATOM 603 C GLY A 785 -21.732 13.831 7.380 1.00 54.77
ATOM 604 O GLY A 785 -20.882 14.378 6.677 1.00 53.15
ATOM 605 N VAL A 786 -21.933 14.152 8.649 1.00 55.12
ATOM 606 CA VAL A 786 -21.147 15.177 9.300 1.00 55.18
ATOM 607 C VAL A 786 -20.685 14.649 10.638 1.00 56.04
ATOM 608 O VAL A 786 -21.445 13.976 11.337 1.00 57.35
ATOM 609 CB VAL A 786 -21.983 16.449 9.546 1.00 55.04
ATOM 610 CG1 VAL A 786 -21.148 17.477 10.282 1.00 54.87
ATOM 611 CG2 VAL A 786 -22.471 17.024 8.226 1.00 54.17
ATOM 612 N CYS A 787 -19.432 14.927 10.982 1.00 56.35
ATOM 613 CA CYS A 787 -18.900 14.517 12.274 1.00 56.07
ATOM 614 C CYS A 787 -18.624 15.800 13.043 1.00 55.27
ATOM 615 O CYS A 787 -17.881 16.661 12.579 1.00 53.31
ATOM 616 CB CYS A 787 -17.608 13.718 12.128 1.00 57.61
ATOM 617 SG CYS A 787 -16.830 13.406 13.747 1.00 65.10

ATOM 618 N LEU A 788 -19.216 15.918 14.222 1.00 56.11
ATOM 619 CA LEU A 788 -19.062 17.115 15.032 1.00 59.11
ATOM 620 C LEU A 788 -17.748 17.221 15.816 1.00 62.37
ATOM 621 O LEU A 788 -17.417 18.290 16.337 1.00 62.61
ATOM 622 CB LEU A 788 -20.250 17.220 15.987 1.00 56.56
ATOM 623 CG LEU A 788 -21.630 17.156 15.312 1.00 56.06
ATOM 624 CD1 LEU A 788 -22.708 17.085 16.375 1.00 53.74
ATOM 625 CD2 LEU A 788 -21.851 18.363 14.409 1.00 53.03
ATOM 626 N SER A 789 -16.991 16.130 15.893 1.00 65.37
ATOM 627 CA SER A 789 -15.732 16.142 16.641 1.00 68.05
ATOM 628 C SER A 789 -14.485 15.926 15.791 1.00 68.52
ATOM 629 O SER A 789 -14.522 15.191 14.805 1.00 69.20
ATOM 630 CB SER A 789 -15.767 15.078 17.739 1.00 68.67
ATOM 631 OG SER A 789 -14.457 14.804 18.207 1.00 72.14
ATOM 632 N PRO A 790 -13.365 16.587 16.154 1.00 69.26
ATOM 633 CA PRO A 790 -13.256 17.506 17.299 1.00 69.34
ATOM 634 C PRO A 790 -13.945 18.796 16.889 1.00 69.49
ATOM 635 O PRO A 790 -14.528 19.515 17.702 1.00 69.32
ATOM 636 CB PRO A 790 -11.750 17.677 17.458 1.00 68.09
ATOM 637 CG PRO A 790 -11.257 17.571 16.042 1.00 68.60
ATOM 638 CD PRO A 790 -12.051 16.403 15.507 1.00 68.85
ATOM 639 N THR A 791 -13.844 19.065 15.595 1.00 69.16
ATOM 640 CA THR A 791 -14.461 20.211 14.964 1.00 69.04
ATOM 641 C THR A 791 -15.183 19.583 13.787 1.00 67.87
ATOM 642 O THR A 791 -14.762 18.547 13.266 1.00 67.60
ATOM 643 CB THR A 791 -13.425 21.225 14.447 1.00 70.57
ATOM 644 OG1 THR A 791 -12.586 20.599 13.466 1.00 70.47
ATOM 645 CG2 THR A 791 -12.577 21.743 15.601 1.00 72.25
ATOM 646 N ILE A 792 -16.275 20.208 13.380 1.00 65.93
ATOM 647 CA ILE A 792 -17.081 19.707 12.288 1.00 63.52
ATOM 648 C ILE A 792 -16.307 19.199 11.082 1.00 61.83
ATOM 649 O ILE A 792 -15.436 19.882 10.551 1.00 60.85
ATOM 650 CB ILE A 792 -18.091 20.771 11.853 1.00 63.29
ATOM 651 CG1 ILE A 792 -19.080 21.014 13.001 1.00 63.31
ATOM 652 CG2 ILE A 792 -18.790 20.323 10.607 1.00 63.07
ATOM 653 CD1 ILE A 792 -20.228 21.943 12.680 1.00 66.80
ATOM 654 N GLN A 793 -16.642 17.983 10.666 1.00 61.24
ATOM 655 CA GLN A 793 -15.999 17.350 9.526 1.00 61.88
ATOM 656 C GLN A 793 -17.060 16.918 8.522 1.00 60.80
ATOM 657 O GLN A 793 -18.049 16.272 8.885 1.00 59.39
ATOM 658 CB GLN A 793 -15.196 16.122 9.968 1.00 63.66
ATOM 659 CG GLN A 793 -14.283 16.345 11.166 1.00 64.96
ATOM 660 CD GLN A 793 -13.435 15.123 11.493 1.00 66.60
ATOM 661 OE1 GLN A 793 -13.341 14.190 10.695 1.00 68.16
ATOM 662 NE2 GLN A 793 -12.824 15.119 12.676 1.00 67.52

```
ATOM    663  N   LEU A 794     -16.841  17.282   7.260  1.00 59.86
ATOM    664  CA  LEU A 794     -17.759  16.946   6.181  1.00 58.57
ATOM    665  C   LEU A 794     -17.334  15.628   5.571  1.00 58.29
ATOM    666  O   LEU A 794     -16.141  15.357   5.441  1.00 58.99
ATOM    667  CB  LEU A 794     -17.747  18.051   5.128  1.00 59.01
ATOM    668  CG  LEU A 794     -18.194  19.414   5.668  1.00 58.65
ATOM    669  CD1 LEU A 794     -18.223  20.438   4.546  1.00 58.33
ATOM    670  CD2 LEU A 794     -19.573  19.276   6.298  1.00 57.68
ATOM    671  N   VAL A 795     -18.311  14.807   5.199  1.00 58.23
ATOM    672  CA  VAL A 795     -18.025  13.493   4.635  1.00 57.20
ATOM    673  C   VAL A 795     -18.868  13.178   3.411  1.00 58.75
ATOM    674  O   VAL A 795     -20.096  13.062   3.490  1.00 57.69
ATOM    675  CB  VAL A 795     -18.257  12.371   5.680  1.00 55.92
ATOM    676  CG1 VAL A 795     -17.708  11.054   5.163  1.00 55.27
ATOM    677  CG2 VAL A 795     -17.604  12.740   7.003  1.00 54.71
ATOM    678  N   THR A 796     -18.184  13.025   2.283  1.00 60.18
ATOM    679  CA  THR A 796     -18.824  12.716   1.018  1.00 63.32
ATOM    680  C   THR A 796     -18.246  11.432   0.461  1.00 64.55
ATOM    681  O   THR A 796     -17.150  11.012   0.838  1.00 64.79
ATOM    682  CB  THR A 796     -18.555  13.799  -0.050  1.00 63.87
ATOM    683  OG1 THR A 796     -18.802  15.099   0.494  1.00 67.06
ATOM    684  CG2 THR A 796     -19.463  13.586  -1.255  1.00 63.95
ATOM    685  N   GLN A 797     -18.991  10.815  -0.445  1.00 65.24
ATOM    686  CA  GLN A 797     -18.522   9.611  -1.100  1.00 66.49
ATOM    687  C   GLN A 797     -17.288  10.093  -1.848  1.00 66.60
ATOM    688  O   GLN A 797     -17.234  11.249  -2.278  1.00 67.28
ATOM    689  CB  GLN A 797     -19.569   9.120  -2.089  1.00 67.59
ATOM    690  CG  GLN A 797     -19.197   7.860  -2.834  1.00 71.35
ATOM    691  CD  GLN A 797     -20.192   7.552  -3.940  1.00 74.61
ATOM    692  OE1 GLN A 797     -21.400   7.453  -3.696  1.00 75.46
ATOM    693  NE2 GLN A 797     -19.693   7.405  -5.166  1.00 74.15
ATOM    694  N   LEU A 798     -16.287   9.234  -1.986  1.00 65.62
ATOM    695  CA  LEU A 798     -15.082   9.631  -2.697  1.00 64.21
ATOM    696  C   LEU A 798     -15.309   9.410  -4.187  1.00 65.69
ATOM    697  O   LEU A 798     -16.029   8.487  -4.582  1.00 66.02
ATOM    698  CB  LEU A 798     -13.888   8.801  -2.228  1.00 61.04
ATOM    699  CG  LEU A 798     -12.541   9.140  -2.860  1.00 60.59
ATOM    700  CD1 LEU A 798     -12.125  10.543  -2.451  1.00 60.17
ATOM    701  CD2 LEU A 798     -11.498   8.133  -2.415  1.00 59.95
ATOM    702  N   MET A 799     -14.722  10.272  -5.013  1.00 65.98
ATOM    703  CA  MET A 799     -14.846  10.135  -6.459  1.00 65.14
ATOM    704  C   MET A 799     -13.531   9.518  -6.915  1.00 64.98
ATOM    705  O   MET A 799     -12.497  10.186  -6.964  1.00 65.11
ATOM    706  CB  MET A 799     -15.076  11.499  -7.123  1.00 64.55
ATOM    707  CG  MET A 799     -16.418  12.140  -6.791  1.00 62.41
```

```
ATOM    708  SD  MET A 799     -17.821  11.182  -7.391  1.00 63.79
ATOM    709  CE  MET A 799     -18.278  10.242  -5.953  1.00 63.53
ATOM    710  N   PRO A 800     -13.559   8.221  -7.249  1.00 65.17
ATOM    711  CA  PRO A 800     -12.386   7.464  -7.697  1.00 65.94
ATOM    712  C   PRO A 800     -11.452   8.149  -8.692  1.00 65.86
ATOM    713  O   PRO A 800     -10.254   8.255  -8.443  1.00 64.64
ATOM    714  CB  PRO A 800     -12.999   6.173  -8.257  1.00 66.48
ATOM    715  CG  PRO A 800     -14.391   6.583  -8.651  1.00 65.65
ATOM    716  CD  PRO A 800     -14.792   7.454  -7.496  1.00 65.28
ATOM    717  N   HIS A 801     -11.998   8.614  -9.811  1.00 66.24
ATOM    718  CA  HIS A 801     -11.185   9.251 -10.834  1.00 66.32
ATOM    719  C   HIS A 801     -10.814  10.712 -10.584  1.00 65.51
ATOM    720  O   HIS A 801     -10.474  11.439 -11.512  1.00 66.97
ATOM    721  CB  HIS A 801     -11.861   9.082 -12.195  1.00 68.47
ATOM    722  CG  HIS A 801     -11.882   7.661 -12.679  1.00 70.66
ATOM    723  ND1 HIS A 801     -10.742   6.990 -13.071  1.00 70.46
ATOM    724  CD2 HIS A 801     -12.900   6.773 -12.798  1.00 71.35
ATOM    725  CE1 HIS A 801     -11.057   5.751 -13.407  1.00 70.98
ATOM    726  NE2 HIS A 801     -12.359   5.593 -13.250  1.00 71.18
ATOM    727  N   GLY A 802     -10.885  11.130  -9.324  1.00 64.19
ATOM    728  CA  GLY A 802     -10.503  12.479  -8.929  1.00 61.92
ATOM    729  C   GLY A 802     -11.137  13.756  -9.473  1.00 60.42
ATOM    730  O   GLY A 802     -12.277  13.794  -9.935  1.00 57.28
ATOM    731  N   CYS A 803     -10.355  14.825  -9.374  1.00 59.58
ATOM    732  CA  CYS A 803     -10.755  16.146  -9.812  1.00 58.64
ATOM    733  C   CYS A 803     -10.613  16.269 -11.316  1.00 59.22
ATOM    734  O   CYS A 803      -9.576  15.912 -11.881  1.00 59.33
ATOM    735  CB  CYS A 803      -9.891  17.202  -9.123  1.00 58.78
ATOM    736  SG  CYS A 803     -10.148  17.335  -7.322  1.00 60.97
ATOM    737  N   LEU A 804     -11.660  16.786 -11.955  1.00 58.47
ATOM    738  CA  LEU A 804     -11.686  16.960 -13.399  1.00 57.67
ATOM    739  C   LEU A 804     -10.524  17.792 -13.938  1.00 57.23
ATOM    740  O   LEU A 804      -9.973  17.494 -14.995  1.00 57.42
ATOM    741  CB  LEU A 804     -13.010  17.592 -13.822  1.00 57.36
ATOM    742  CG  LEU A 804     -13.136  17.853 -15.323  1.00 56.02
ATOM    743  CD1 LEU A 804     -12.864  16.566 -16.073  1.00 56.06
ATOM    744  CD2 LEU A 804     -14.522  18.392 -15.646  1.00 56.14
ATOM    745  N   LEU A 805     -10.151  18.839 -13.219  1.00 56.60
ATOM    746  CA  LEU A 805      -9.054  19.674 -13.666  1.00 57.25
ATOM    747  C   LEU A 805      -7.770  18.871 -13.836  1.00 59.50
ATOM    748  O   LEU A 805      -7.068  19.041 -14.826  1.00 61.05
ATOM    749  CB  LEU A 805      -8.821  20.814 -12.681  1.00 54.99
ATOM    750  CG  LEU A 805      -7.600  21.668 -12.995  1.00 52.96
ATOM    751  CD1 LEU A 805      -7.614  22.102 -14.453  1.00 51.15
ATOM    752  CD2 LEU A 805      -7.596  22.863 -12.072  1.00 53.82
```

```
ATOM   753  N   GLU A 806     -7.458  18.006 -12.873  1.00 61.71
ATOM   754  CA  GLU A 806     -6.249  17.186 -12.952  1.00 64.25
ATOM   755  C   GLU A 806     -6.435  16.119 -14.027  1.00 63.97
ATOM   756  O   GLU A 806     -5.477  15.676 -14.665  1.00 63.45
ATOM   757  CB  GLU A 806     -5.957  16.495 -11.611  1.00 67.06
ATOM   758  CG  GLU A 806     -5.509  17.425 -10.477  1.00 73.60
ATOM   759  CD  GLU A 806     -5.169  16.666  -9.188  1.00 76.72
ATOM   760  OE1 GLU A 806     -5.484  15.455  -9.105  1.00 77.37
ATOM   761  OE2 GLU A 806     -4.593  17.279  -8.259  1.00 78.10
ATOM   762  N   TYR A 807     -7.684  15.719 -14.228  1.00 63.27
ATOM   763  CA  TYR A 807     -8.015  14.694 -15.203  1.00 63.32
ATOM   764  C   TYR A 807     -7.749  15.098 -16.649  1.00 62.69
ATOM   765  O   TYR A 807     -7.050  14.391 -17.364  1.00 61.57
ATOM   766  CB  TYR A 807     -9.478  14.294 -15.058  1.00 63.62
ATOM   767  CG  TYR A 807     -9.822  13.015 -15.769  1.00 63.28
ATOM   768  CD1 TYR A 807     -9.545  11.778 -15.189  1.00 62.76
ATOM   769  CD2 TYR A 807    -10.436  13.040 -17.017  1.00 63.66
ATOM   770  CE1 TYR A 807     -9.879  10.597 -15.834  1.00 63.41
ATOM   771  CE2 TYR A 807    -10.771  11.867 -17.671  1.00 64.64
ATOM   772  CZ  TYR A 807    -10.494  10.650 -17.074  1.00 64.30
ATOM   773  OH  TYR A 807    -10.854   9.494 -17.719  1.00 65.98
ATOM   774  N   VAL A 808     -8.305  16.223 -17.087  1.00 62.57
ATOM   775  CA  VAL A 808     -8.087  16.644 -18.466  1.00 64.21
ATOM   776  C   VAL A 808     -6.626  16.901 -18.773  1.00 65.63
ATOM   777  O   VAL A 808     -6.238  16.927 -19.933  1.00 66.29
ATOM   778  CB  VAL A 808     -8.865  17.914 -18.831  1.00 61.95
ATOM   779  CG1 VAL A 808    -10.337  17.614 -18.891  1.00 61.31
ATOM   780  CG2 VAL A 808     -8.568  19.003 -17.832  1.00 61.93
ATOM   781  N   HIS A 809     -5.811  17.093 -17.746  1.00 68.17
ATOM   782  CA  HIS A 809     -4.398  17.337 -17.986  1.00 72.57
ATOM   783  C   HIS A 809     -3.690  16.011 -18.246  1.00 72.86
ATOM   784  O   HIS A 809     -3.024  15.834 -19.266  1.00 73.15
ATOM   785  CB  HIS A 809     -3.756  18.034 -16.787  1.00 76.24
ATOM   786  CG  HIS A 809     -2.334  18.446 -17.018  1.00 80.69
ATOM   787  ND1 HIS A 809     -1.989  19.505 -17.831  1.00 82.82
ATOM   788  CD2 HIS A 809     -1.169  17.940 -16.544  1.00 82.57
ATOM   789  CE1 HIS A 809     -0.673  19.635 -17.846  1.00 83.54
ATOM   790  NE2 HIS A 809     -0.152  18.698 -17.074  1.00 83.63
ATOM   791  N   GLU A 810     -3.851  15.077 -17.320  1.00 73.25
ATOM   792  CA  GLU A 810     -3.220  13.776 -17.441  1.00 74.27
ATOM   793  C   GLU A 810     -3.700  12.994 -18.655  1.00 73.56
ATOM   794  O   GLU A 810     -2.901  12.341 -19.331  1.00 73.89
ATOM   795  CB  GLU A 810     -3.466  12.963 -16.172  1.00 76.41
ATOM   796  CG  GLU A 810     -2.767  13.517 -14.941  1.00 80.78
ATOM   797  CD  GLU A 810     -3.185  12.795 -13.670  1.00 84.23
```

```
ATOM    798  OE1 GLU A 810     -3.195  11.542 -13.672  1.00 85.68
ATOM    799  OE2 GLU A 810     -3.498  13.479 -12.668  1.00 84.74
ATOM    800  N   HIS A 811     -4.998  13.070 -18.937  1.00 72.66
ATOM    801  CA  HIS A 811     -5.582  12.346 -20.063  1.00 72.30
ATOM    802  C   HIS A 811     -5.823  13.195 -21.303  1.00 72.06
ATOM    803  O   HIS A 811     -6.591  12.801 -22.187  1.00 71.12
ATOM    804  CB  HIS A 811     -6.899  11.701 -19.638  1.00 73.09
ATOM    805  CG  HIS A 811     -6.750  10.700 -18.539  1.00 74.95
ATOM    806  ND1 HIS A 811     -6.018  10.951 -17.399  1.00 76.95
ATOM    807  CD2 HIS A 811     -7.260   9.455 -18.392  1.00 76.68
ATOM    808  CE1 HIS A 811     -6.084   9.904 -16.596  1.00 77.89
ATOM    809  NE2 HIS A 811     -6.833   8.983 -17.175  1.00 77.93
ATOM    810  N   LYS A 812     -5.167  14.351 -21.369  1.00 72.19
ATOM    811  CA  LYS A 812     -5.321  15.247 -22.510  1.00 72.68
ATOM    812  C   LYS A 812     -5.330  14.462 -23.805  1.00 73.33
ATOM    813  O   LYS A 812     -6.280  14.518 -24.584  1.00 73.60
ATOM    814  CB  LYS A 812     -4.180  16.271 -22.570  1.00 72.21
ATOM    815  CG  LYS A 812     -4.116  16.982 -23.917  1.00 71.18
ATOM    816  CD  LYS A 812     -3.146  18.148 -23.951  1.00 70.28
ATOM    817  CE  LYS A 812     -3.235  18.834 -25.308  1.00 68.88
ATOM    818  NZ  LYS A 812     -2.481  20.108 -25.344  1.00 68.31
ATOM    819  N   ASP A 813     -4.256  13.717 -24.015  1.00 75.12
ATOM    820  CA  ASP A 813     -4.092  12.917 -25.213  1.00 76.11
ATOM    821  C   ASP A 813     -5.038  11.712 -25.213  1.00 75.70
ATOM    822  O   ASP A 813     -4.692  10.641 -25.697  1.00 75.57
ATOM    823  CB  ASP A 813     -2.627  12.469 -25.312  1.00 78.16
ATOM    824  CG  ASP A 813     -1.639  13.629 -25.104  1.00 79.48
ATOM    825  OD1 ASP A 813     -1.703  14.618 -25.867  1.00 78.24
ATOM    826  OD2 ASP A 813     -0.795  13.554 -24.176  1.00 81.15
ATOM    827  N   ASN A 814     -6.237  11.901 -24.671  1.00 75.59
ATOM    828  CA  ASN A 814     -7.232  10.835 -24.609  1.00 75.15
ATOM    829  C   ASN A 814     -8.639  11.421 -24.602  1.00 73.09
ATOM    830  O   ASN A 814     -9.629  10.690 -24.620  1.00 72.17
ATOM    831  CB  ASN A 814     -7.038  10.003 -23.340  1.00 79.73
ATOM    832  CG  ASN A 814     -8.095   8.910 -23.182  1.00 83.39
ATOM    833  OD1 ASN A 814     -8.417   8.495 -22.059  1.00 85.44
ATOM    834  ND2 ASN A 814     -8.628   8.429 -24.306  1.00 82.76
ATOM    835  N   ILE A 815     -8.725  12.746 -24.575  1.00 70.07
ATOM    836  CA  ILE A 815    -10.018  13.414 -24.543  1.00 66.45
ATOM    837  C   ILE A 815    -10.548  13.773 -25.923  1.00 64.58
ATOM    838  O   ILE A 815     -9.910  14.515 -26.670  1.00 65.16
ATOM    839  CB  ILE A 815     -9.940  14.686 -23.701  1.00 66.17
ATOM    840  CG1 ILE A 815     -9.416  14.337 -22.310  1.00 64.41
ATOM    841  CG2 ILE A 815    -11.308  15.341 -23.616  1.00 65.95
ATOM    842  CD1 ILE A 815    -10.283  13.377 -21.576  1.00 64.44
```

```
ATOM    843  N   GLY A 816     -11.727  13.244 -26.244  1.00 61.95
ATOM    844  CA  GLY A 816     -12.348  13.502 -27.529  1.00 58.49
ATOM    845  C   GLY A 816     -13.391  14.602 -27.474  1.00 57.57
ATOM    846  O   GLY A 816     -13.798  15.049 -26.400  1.00 56.05
ATOM    847  N   SER A 817     -13.836  15.036 -28.645  1.00 55.76
ATOM    848  CA  SER A 817     -14.814  16.100 -28.723  1.00 54.42
ATOM    849  C   SER A 817     -16.087  15.748 -27.976  1.00 53.51
ATOM    850  O   SER A 817     -16.653  16.588 -27.277  1.00 53.70
ATOM    851  CB  SER A 817     -15.140  16.417 -30.188  1.00 54.21
ATOM    852  OG  SER A 817     -15.754  15.315 -30.830  1.00 53.76
ATOM    853  N   GLN A 818     -16.526  14.503 -28.118  1.00 52.59
ATOM    854  CA  GLN A 818     -17.755  14.046 -27.481  1.00 52.58
ATOM    855  C   GLN A 818     -17.711  14.105 -25.962  1.00 52.52
ATOM    856  O   GLN A 818     -18.606  14.649 -25.316  1.00 53.30
ATOM    857  CB  GLN A 818     -18.071  12.624 -27.929  1.00 52.77
ATOM    858  CG  GLN A 818     -19.386  12.096 -27.396  1.00 55.94
ATOM    859  CD  GLN A 818     -19.734  10.728 -27.960  1.00 57.95
ATOM    860  OE1 GLN A 818     -19.015   9.749 -27.741  1.00 55.96
ATOM    861  NE2 GLN A 818     -20.841  10.657 -28.694  1.00 58.90
ATOM    862  N   LEU A 819     -16.663  13.535 -25.392  1.00 52.33
ATOM    863  CA  LEU A 819     -16.487  13.519 -23.951  1.00 53.05
ATOM    864  C   LEU A 819     -16.530  14.955 -23.374  1.00 52.97
ATOM    865  O   LEU A 819     -17.199  15.211 -22.372  1.00 51.99
ATOM    866  CB  LEU A 819     -15.147  12.846 -23.641  1.00 55.20
ATOM    867  CG  LEU A 819     -14.857  12.305 -22.246  1.00 58.07
ATOM    868  CD1 LEU A 819     -15.883  11.248 -21.893  1.00 59.70
ATOM    869  CD2 LEU A 819     -13.454  11.722 -22.216  1.00 57.59
ATOM    870  N   LEU A 820     -15.823  15.881 -24.024  1.00 51.18
ATOM    871  CA  LEU A 820     -15.761  17.274 -23.592  1.00 49.17
ATOM    872  C   LEU A 820     -17.089  18.021 -23.663  1.00 48.89
ATOM    873  O   LEU A 820     -17.395  18.820 -22.776  1.00 48.95
ATOM    874  CB  LEU A 820     -14.725  18.041 -24.415  1.00 48.36
ATOM    875  CG  LEU A 820     -13.252  17.791 -24.106  1.00 47.62
ATOM    876  CD1 LEU A 820     -12.411  18.277 -25.275  1.00 47.48
ATOM    877  CD2 LEU A 820     -12.859  18.485 -22.813  1.00 46.35
ATOM    878  N   LEU A 821     -17.867  17.794 -24.719  1.00 47.18
ATOM    879  CA  LEU A 821     -19.158  18.470 -24.845  1.00 45.74
ATOM    880  C   LEU A 821     -20.174  17.912 -23.858  1.00 44.93
ATOM    881  O   LEU A 821     -21.035  18.636 -23.366  1.00 44.43
ATOM    882  CB  LEU A 821     -19.699  18.350 -26.269  1.00 43.56
ATOM    883  CG  LEU A 821     -19.043  19.245 -27.324  1.00 44.32
ATOM    884  CD1 LEU A 821     -19.595  18.904 -28.686  1.00 42.72
ATOM    885  CD2 LEU A 821     -19.299  20.706 -27.015  1.00 41.61
ATOM    886  N   ASN A 822     -20.074  16.620 -23.575  1.00 45.14
ATOM    887  CA  ASN A 822     -20.978  15.992 -22.630  1.00 46.84
```

ATOM 888 C ASN A 822 -20.710 16.514 -21.216 1.00 46.44
ATOM 889 O ASN A 822 -21.629 16.712 -20.429 1.00 47.65
ATOM 890 CB ASN A 822 -20.803 14.480 -22.683 1.00 50.43
ATOM 891 CG ASN A 822 -21.407 13.874 -23.930 1.00 53.27
ATOM 892 OD1 ASN A 822 -22.624 13.914 -24.127 1.00 55.44
ATOM 893 ND2 ASN A 822 -20.564 13.310 -24.782 1.00 55.67
ATOM 894 N TRP A 823 -19.448 16.736 -20.886 1.00 44.44
ATOM 895 CA TRP A 823 -19.126 17.265 -19.571 1.00 44.31
ATOM 896 C TRP A 823 -19.734 18.662 -19.418 1.00 42.62
ATOM 897 O TRP A 823 -20.172 19.051 -18.331 1.00 41.36
ATOM 898 CB TRP A 823 -17.609 17.334 -19.376 1.00 44.91
ATOM 899 CG TRP A 823 -16.949 15.987 -19.186 1.00 46.37
ATOM 900 CD1 TRP A 823 -17.551 14.826 -18.785 1.00 45.40
ATOM 901 CD2 TRP A 823 -15.552 15.689 -19.318 1.00 46.95
ATOM 902 NE1 TRP A 823 -16.615 13.828 -18.656 1.00 46.44
ATOM 903 CE2 TRP A 823 -15.380 14.328 -18.977 1.00 46.59
ATOM 904 CE3 TRP A 823 -14.425 16.441 -19.693 1.00 49.03
ATOM 905 CZ2 TRP A 823 -14.128 13.699 -18.998 1.00 46.68
ATOM 906 CZ3 TRP A 823 -13.169 15.808 -19.715 1.00 50.33
ATOM 907 CH2 TRP A 823 -13.038 14.451 -19.368 1.00 47.90
ATOM 908 N CYS A 824 -19.773 19.407 -20.514 1.00 40.45
ATOM 909 CA CYS A 824 -20.329 20.746 -20.489 1.00 42.24
ATOM 910 C CYS A 824 -21.799 20.690 -20.146 1.00 43.66
ATOM 911 O CYS A 824 -22.309 21.548 -19.426 1.00 43.87
ATOM 912 CB CYS A 824 -20.138 21.439 -21.836 1.00 43.69
ATOM 913 SG CYS A 824 -18.428 21.910 -22.159 1.00 44.22
ATOM 914 N VAL A 825 -22.472 19.668 -20.667 1.00 45.00
ATOM 915 CA VAL A 825 -23.896 19.459 -20.425 1.00 42.03
ATOM 916 C VAL A 825 -24.109 19.061 -18.973 1.00 42.11
ATOM 917 O VAL A 825 -24.921 19.653 -18.254 1.00 40.65
ATOM 918 CB VAL A 825 -24.441 18.353 -21.337 1.00 41.91
ATOM 919 CG1 VAL A 825 -25.865 17.993 -20.940 1.00 41.30
ATOM 920 CG2 VAL A 825 -24.392 18.821 -22.788 1.00 41.84
ATOM 921 N GLN A 826 -23.362 18.053 -18.543 1.00 42.60
ATOM 922 CA GLN A 826 -23.460 17.573 -17.175 1.00 42.94
ATOM 923 C GLN A 826 -23.232 18.697 -16.182 1.00 40.98
ATOM 924 O GLN A 826 -24.012 18.858 -15.253 1.00 41.31
ATOM 925 CB GLN A 826 -22.475 16.428 -16.965 1.00 43.82
ATOM 926 CG GLN A 826 -22.954 15.187 -17.689 1.00 46.63
ATOM 927 CD GLN A 826 -21.996 14.029 -17.594 1.00 47.66
ATOM 928 OE1 GLN A 826 -21.205 13.938 -16.660 1.00 47.25
ATOM 929 NE2 GLN A 826 -22.077 13.119 -18.559 1.00 49.33
ATOM 930 N ILE A 827 -22.180 19.485 -16.381 1.00 39.59
ATOM 931 CA ILE A 827 -21.920 20.598 -15.479 1.00 38.36
ATOM 932 C ILE A 827 -23.090 21.596 -15.527 1.00 39.97

ATOM 933 O ILE A 827 -23.643 21.967 -14.485 1.00 41.14
ATOM 934 CB ILE A 827 -20.607 21.329 -15.834 1.00 36.75
ATOM 935 CG1 ILE A 827 -19.449 20.320 -15.852 1.00 36.42
ATOM 936 CG2 ILE A 827 -20.335 22.436 -14.816 1.00 32.91
ATOM 937 CD1 ILE A 827 -18.064 20.930 -15.996 1.00 33.58
ATOM 938 N ALA A 828 -23.479 22.016 -16.727 1.00 38.03
ATOM 939 CA ALA A 828 -24.581 22.957 -16.867 1.00 38.98
ATOM 940 C ALA A 828 -25.848 22.407 -16.203 1.00 41.61
ATOM 941 O ALA A 828 -26.562 23.133 -15.514 1.00 41.11
ATOM 942 CB ALA A 828 -24.835 23.253 -18.339 1.00 37.80
ATOM 943 N LYS A 829 -26.120 21.118 -16.398 1.00 43.40
ATOM 944 CA LYS A 829 -27.302 20.502 -15.803 1.00 43.58
ATOM 945 C LYS A 829 -27.298 20.557 -14.277 1.00 45.12
ATOM 946 O LYS A 829 -28.319 20.849 -13.666 1.00 45.69
ATOM 947 CB LYS A 829 -27.444 19.055 -16.272 1.00 43.15
ATOM 948 CG LYS A 829 -28.315 18.892 -17.508 1.00 43.32
ATOM 949 CD LYS A 829 -28.403 17.433 -17.912 1.00 47.16
ATOM 950 CE LYS A 829 -29.243 17.228 -19.164 1.00 49.43
ATOM 951 NZ LYS A 829 -29.209 15.792 -19.577 1.00 50.93
ATOM 952 N GLY A 830 -26.159 20.268 -13.661 1.00 46.16
ATOM 953 CA GLY A 830 -26.090 20.327 -12.214 1.00 46.02
ATOM 954 C GLY A 830 -26.349 21.744 -11.721 1.00 46.34
ATOM 955 O GLY A 830 -27.060 21.948 -10.729 1.00 46.09
ATOM 956 N MET A 831 -25.770 22.731 -12.399 1.00 45.04
ATOM 957 CA MET A 831 -25.982 24.119 -11.999 1.00 46.30
ATOM 958 C MET A 831 -27.484 24.407 -12.125 1.00 47.00
ATOM 959 O MET A 831 -28.076 25.117 -11.306 1.00 45.79
ATOM 960 CB MET A 831 -25.173 25.069 -12.896 1.00 43.99
ATOM 961 CG MET A 831 -23.675 24.923 -12.748 1.00 40.18
ATOM 962 SD MET A 831 -23.169 25.141 -11.023 1.00 41.93
ATOM 963 CE MET A 831 -23.711 26.840 -10.757 1.00 41.68
ATOM 964 N MET A 832 -28.084 23.819 -13.156 1.00 46.35
ATOM 965 CA MET A 832 -29.503 23.954 -13.444 1.00 48.31
ATOM 966 C MET A 832 -30.330 23.517 -12.236 1.00 47.54
ATOM 967 O MET A 832 -31.274 24.197 -11.828 1.00 49.03
ATOM 968 CB MET A 832 -29.835 23.080 -14.648 1.00 52.33
ATOM 969 CG MET A 832 -31.143 23.377 -15.345 1.00 57.13
ATOM 970 SD MET A 832 -31.249 22.334 -16.823 1.00 62.53
ATOM 971 CE MET A 832 -30.102 23.157 -17.832 1.00 58.95
ATOM 972 N TYR A 833 -29.963 22.375 -11.670 1.00 45.22
ATOM 973 CA TYR A 833 -30.637 21.832 -10.508 1.00 43.85
ATOM 974 C TYR A 833 -30.446 22.781 -9.332 1.00 45.57
ATOM 975 O TYR A 833 -31.382 23.033 -8.571 1.00 44.47
ATOM 976 CB TYR A 833 -30.041 20.475 -10.161 1.00 42.10
ATOM 977 CG TYR A 833 -30.709 19.759 -9.006 1.00 42.47

ATOM 978 CD1 TYR A 833 -31.781 18.877 -9.223 1.00 41.47
ATOM 979 CD2 TYR A 833 -30.226 19.902 -7.702 1.00 39.44
ATOM 980 CE1 TYR A 833 -32.344 18.143 -8.165 1.00 37.67
ATOM 981 CE2 TYR A 833 -30.784 19.184 -6.639 1.00 39.15
ATOM 982 CZ TYR A 833 -31.837 18.306 -6.877 1.00 38.87
ATOM 983 OH TYR A 833 -32.378 17.600 -5.827 1.00 38.16
ATOM 984 N LEU A 834 -29.232 23.304 -9.176 1.00 45.55
ATOM 985 CA LEU A 834 -28.958 24.225 -8.072 1.00 46.56
ATOM 986 C LEU A 834 -29.800 25.496 -8.168 1.00 45.77
ATOM 987 O LEU A 834 -30.432 25.894 -7.199 1.00 45.06
ATOM 988 CB LEU A 834 -27.468 24.601 -8.022 1.00 46.73
ATOM 989 CG LEU A 834 -26.445 23.528 -7.609 1.00 47.94
ATOM 990 CD1 LEU A 834 -25.044 24.081 -7.736 1.00 45.98
ATOM 991 CD2 LEU A 834 -26.679 23.094 -6.184 1.00 46.82
ATOM 992 N GLU A 835 -29.803 26.126 -9.337 1.00 46.46
ATOM 993 CA GLU A 835 -30.561 27.359 -9.559 1.00 48.02
ATOM 994 C GLU A 835 -32.059 27.172 -9.298 1.00 48.70
ATOM 995 O GLU A 835 -32.749 28.101 -8.872 1.00 44.97
ATOM 996 CB GLU A 835 -30.357 27.835 -10.997 1.00 48.88
ATOM 997 CG GLU A 835 -30.994 29.167 -11.320 1.00 51.38
ATOM 998 CD GLU A 835 -30.899 29.497 -12.791 1.00 55.29
ATOM 999 OE1 GLU A 835 -31.031 30.682 -13.160 1.00 61.79
ATOM 1000 OE2 GLU A 835 -30.699 28.562 -13.591 1.00 59.22
ATOM 1001 N GLU A 836 -32.547 25.966 -9.585 1.00 49.61
ATOM 1002 CA GLU A 836 -33.941 25.609 -9.393 1.00 51.33
ATOM 1003 C GLU A 836 -34.251 25.644 -7.893 1.00 52.42
ATOM 1004 O GLU A 836 -35.376 25.933 -7.476 1.00 53.59
ATOM 1005 CB GLU A 836 -34.172 24.213 -9.976 1.00 53.43
ATOM 1006 CG GLU A 836 -35.554 23.632 -9.752 1.00 61.91
ATOM 1007 CD GLU A 836 -35.694 22.222 -10.322 1.00 68.30
ATOM 1008 OE1 GLU A 836 -34.777 21.393 -10.103 1.00 70.37
ATOM 1009 OE2 GLU A 836 -36.723 21.938 -10.984 1.00 72.73
ATOM 1010 N ARG A 837 -33.232 25.366 -7.089 1.00 52.07
ATOM 1011 CA ARG A 837 -33.342 25.363 -5.632 1.00 53.28
ATOM 1012 C ARG A 837 -32.980 26.731 -5.018 1.00 53.42
ATOM 1013 O ARG A 837 -32.909 26.859 -3.800 1.00 52.59
ATOM 1014 CB ARG A 837 -32.401 24.300 -5.041 1.00 54.24
ATOM 1015 CG ARG A 837 -32.654 22.870 -5.507 1.00 54.61
ATOM 1016 CD ARG A 837 -33.996 22.419 -5.013 1.00 54.07
ATOM 1017 NE ARG A 837 -34.338 21.032 -5.316 1.00 54.63
ATOM 1018 CZ ARG A 837 -34.342 20.493 -6.529 1.00 53.35
ATOM 1019 NH1 ARG A 837 -33.993 21.207 -7.590 1.00 54.44
ATOM 1020 NH2 ARG A 837 -34.777 19.250 -6.687 1.00 52.90
ATOM 1021 N ARG A 838 -32.739 27.734 -5.862 1.00 54.60
ATOM 1022 CA ARG A 838 -32.366 29.084 -5.417 1.00 56.39

```
ATOM  1023  C   ARG A 838    -30.963  29.097  -4.789  1.00 55.44
ATOM  1024  O   ARG A 838    -30.669  29.912  -3.911  1.00 55.30
ATOM  1025  CB  ARG A 838    -33.378  29.619  -4.393  1.00 60.89
ATOM  1026  CG  ARG A 838    -34.852  29.577  -4.822  1.00 68.36
ATOM  1027  CD  ARG A 838    -35.206  30.654  -5.846  1.00 73.13
ATOM  1028  NE  ARG A 838    -36.650  30.723  -6.105  1.00 77.28
ATOM  1029  CZ  ARG A 838    -37.320  29.908  -6.920  1.00 78.68
ATOM  1030  NH1 ARG A 838    -38.629  30.061  -7.074  1.00 78.70
ATOM  1031  NH2 ARG A 838    -36.686  28.951  -7.592  1.00 78.88
ATOM  1032  N   LEU A 839    -30.091  28.207  -5.253  1.00 52.78
ATOM  1033  CA  LEU A 839    -28.744  28.115  -4.703  1.00 50.80
ATOM  1034  C   LEU A 839    -27.635  28.587  -5.644  1.00 49.61
ATOM  1035  O   LEU A 839    -27.558  28.180  -6.801  1.00 51.46
ATOM  1036  CB  LEU A 839    -28.472  26.674  -4.275  1.00 51.33
ATOM  1037  CG  LEU A 839    -29.535  26.036  -3.370  1.00 52.40
ATOM  1038  CD1 LEU A 839    -29.216  24.548  -3.176  1.00 51.01
ATOM  1039  CD2 LEU A 839    -29.593  26.778  -2.026  1.00 50.05
ATOM  1040  N   VAL A 840    -26.773  29.455  -5.138  1.00 46.94
ATOM  1041  CA  VAL A 840    -25.671  29.958  -5.933  1.00 45.16
ATOM  1042  C   VAL A 840    -24.388  29.267  -5.497  1.00 45.42
ATOM  1043  O   VAL A 840    -24.124  29.147  -4.309  1.00 45.89
ATOM  1044  CB  VAL A 840    -25.515  31.472  -5.750  1.00 44.00
ATOM  1045  CG1 VAL A 840    -24.412  32.005  -6.673  1.00 39.24
ATOM  1046  CG2 VAL A 840    -26.846  32.150  -6.036  1.00 42.54
ATOM  1047  N   HIS A 841    -23.588  28.805  -6.450  1.00 45.68
ATOM  1048  CA  HIS A 841    -22.343  28.137  -6.097  1.00 45.32
ATOM  1049  C   HIS A 841    -21.307  29.133  -5.578  1.00 45.51
ATOM  1050  O   HIS A 841    -20.752  28.958  -4.496  1.00 46.26
ATOM  1051  CB  HIS A 841    -21.778  27.396  -7.305  1.00 44.31
ATOM  1052  CG  HIS A 841    -20.707  26.410  -6.956  1.00 43.65
ATOM  1053  ND1 HIS A 841    -19.583  26.755  -6.240  1.00 41.64
ATOM  1054  CD2 HIS A 841    -20.592  25.088  -7.222  1.00 43.78
ATOM  1055  CE1 HIS A 841    -18.821  25.689  -6.080  1.00 42.85
ATOM  1056  NE2 HIS A 841    -19.410  24.664  -6.667  1.00 43.25
ATOM  1057  N   ARG A 842    -21.050  30.173  -6.363  1.00 46.38
ATOM  1058  CA  ARG A 842    -20.086  31.213  -6.009  1.00 48.44
ATOM  1059  C   ARG A 842    -18.643  30.854  -6.304  1.00 47.29
ATOM  1060  O   ARG A 842    -17.800  31.737  -6.407  1.00 47.23
ATOM  1061  CB  ARG A 842    -20.199  31.600  -4.533  1.00 50.08
ATOM  1062  CG  ARG A 842    -21.388  32.452  -4.221  1.00 55.04
ATOM  1063  CD  ARG A 842    -21.436  32.802  -2.759  1.00 59.44
ATOM  1064  NE  ARG A 842    -22.511  33.746  -2.470  1.00 62.17
ATOM  1065  CZ  ARG A 842    -22.698  34.317  -1.286  1.00 63.69
ATOM  1066  NH1 ARG A 842    -21.881  34.037  -0.282  1.00 65.35
ATOM  1067  NH2 ARG A 842    -23.699  35.166  -1.106  1.00 64.62
```

```
ATOM   1068  N   ASP A 843     -18.349  29.568  -6.440  1.00 46.08
ATOM   1069  CA  ASP A 843     -16.978  29.160  -6.714  1.00 44.50
ATOM   1070  C   ASP A 843     -16.877  27.969  -7.671  1.00 42.28
ATOM   1071  O   ASP A 843     -16.163  26.997  -7.412  1.00 39.78
ATOM   1072  CB  ASP A 843     -16.260  28.857  -5.393  1.00 44.95
ATOM   1073  CG  ASP A 843     -14.794  28.536  -5.588  1.00 45.84
ATOM   1074  OD1 ASP A 843     -14.145  29.230  -6.403  1.00 47.66
ATOM   1075  OD2 ASP A 843     -14.293  27.600  -4.925  1.00 44.46
ATOM   1076  N   LEU A 844     -17.601  28.052  -8.781  1.00 39.91
ATOM   1077  CA  LEU A 844     -17.569  26.997  -9.774  1.00 38.68
ATOM   1078  C   LEU A 844     -16.267  27.143 -10.579  1.00 39.36
ATOM   1079  O   LEU A 844     -15.909  28.244 -11.012  1.00 36.39
ATOM   1080  CB  LEU A 844     -18.787  27.110 -10.690  1.00 37.44
ATOM   1081  CG  LEU A 844     -18.818  26.190 -11.918  1.00 35.03
ATOM   1082  CD1 LEU A 844     -18.793  24.735 -11.502  1.00 33.46
ATOM   1083  CD2 LEU A 844     -20.061  26.486 -12.710  1.00 33.77
ATOM   1084  N   ALA A 845     -15.554  26.035 -10.749  1.00 38.08
ATOM   1085  CA  ALA A 845     -14.294  26.041 -11.481  1.00 41.74
ATOM   1086  C   ALA A 845     -13.890  24.602 -11.766  1.00 43.66
ATOM   1087  O   ALA A 845     -14.272  23.692 -11.029  1.00 45.06
ATOM   1088  CB  ALA A 845     -13.209  26.740 -10.653  1.00 41.01
ATOM   1089  N   ALA A 846     -13.128  24.388 -12.832  1.00 45.09
ATOM   1090  CA  ALA A 846     -12.706  23.034 -13.183  1.00 46.69
ATOM   1091  C   ALA A 846     -12.244  22.297 -11.933  1.00 47.45
ATOM   1092  O   ALA A 846     -12.454  21.094 -11.789  1.00 49.65
ATOM   1093  CB  ALA A 846     -11.591  23.083 -14.208  1.00 45.74
ATOM   1094  N   ARG A 847     -11.632  23.047 -11.027  1.00 49.09
ATOM   1095  CA  ARG A 847     -11.117  22.527  -9.759  1.00 50.53
ATOM   1096  C   ARG A 847     -12.175  21.893  -8.858  1.00 50.50
ATOM   1097  O   ARG A 847     -11.872  20.978  -8.100  1.00 51.14
ATOM   1098  CB  ARG A 847     -10.421  23.664  -9.015  1.00 52.11
ATOM   1099  CG  ARG A 847     -10.116  23.414  -7.567  1.00 55.22
ATOM   1100  CD  ARG A 847      -9.438  24.635  -7.002  1.00 54.87
ATOM   1101  NE  ARG A 847     -10.266  25.814  -7.214  1.00 59.60
ATOM   1102  CZ  ARG A 847     -11.222  26.221  -6.381  1.00 62.29
ATOM   1103  NH1 ARG A 847     -11.468  25.543  -5.262  1.00 63.16
ATOM   1104  NH2 ARG A 847     -11.942  27.298  -6.676  1.00 61.26
ATOM   1105  N   ASN A 848     -13.412  22.374  -8.931  1.00 49.43
ATOM   1106  CA  ASN A 848     -14.469  21.819  -8.099  1.00 47.44
ATOM   1107  C   ASN A 848     -15.438  20.903  -8.840  1.00 48.04
ATOM   1108  O   ASN A 848     -16.612  20.784  -8.472  1.00 48.54
ATOM   1109  CB  ASN A 848     -15.236  22.934  -7.384  1.00 45.48
ATOM   1110  CG  ASN A 848     -14.397  23.628  -6.337  1.00 45.91
ATOM   1111  OD1 ASN A 848     -13.754  22.979  -5.521  1.00 50.11
ATOM   1112  ND2 ASN A 848     -14.406  24.950  -6.347  1.00 43.85
```

ATOM 1113 N VAL A 849 -14.951 20.265 -9.897 1.00 46.96
ATOM 1114 CA VAL A 849 -15.771 19.318 -10.637 1.00 47.48
ATOM 1115 C VAL A 849 -15.026 17.994 -10.477 1.00 48.51
ATOM 1116 O VAL A 849 -13.826 17.913 -10.729 1.00 49.29
ATOM 1117 CB VAL A 849 -15.896 19.688 -12.145 1.00 47.07
ATOM 1118 CG1 VAL A 849 -16.754 18.653 -12.871 1.00 47.56
ATOM 1119 CG2 VAL A 849 -16.517 21.065 -12.298 1.00 45.99
ATOM 1120 N LEU A 850 -15.730 16.965 -10.026 1.00 48.67
ATOM 1121 CA LEU A 850 -15.109 15.667 -9.813 1.00 47.31
ATOM 1122 C LEU A 850 -15.554 14.634 -10.855 1.00 48.46
ATOM 1123 O LEU A 850 -16.641 14.733 -11.430 1.00 47.00
ATOM 1124 CB LEU A 850 -15.437 15.165 -8.402 1.00 43.85
ATOM 1125 CG LEU A 850 -15.177 16.144 -7.255 1.00 42.97
ATOM 1126 CD1 LEU A 850 -15.709 15.561 -5.970 1.00 40.25
ATOM 1127 CD2 LEU A 850 -13.694 16.439 -7.137 1.00 42.26
ATOM 1128 N VAL A 851 -14.701 13.638 -11.082 1.00 50.16
ATOM 1129 CA VAL A 851 -14.985 12.588 -12.045 1.00 51.71
ATOM 1130 C VAL A 851 -15.343 11.257 -11.371 1.00 54.08
ATOM 1131 O VAL A 851 -14.485 10.615 -10.757 1.00 53.24
ATOM 1132 CB VAL A 851 -13.772 12.355 -12.963 1.00 51.18
ATOM 1133 CG1 VAL A 851 -14.208 11.572 -14.195 1.00 53.03
ATOM 1134 CG2 VAL A 851 -13.136 13.683 -13.351 1.00 48.08
ATOM 1135 N LYS A 852 -16.610 10.854 -11.473 1.00 56.51
ATOM 1136 CA LYS A 852 -17.060 9.581 -10.897 1.00 60.15
ATOM 1137 C LYS A 852 -16.552 8.520 -11.863 1.00 62.24
ATOM 1138 O LYS A 852 -16.067 7.461 -11.464 1.00 64.74
ATOM 1139 CB LYS A 852 -18.584 9.524 -10.829 1.00 60.47
ATOM 1140 CG LYS A 852 -19.156 8.246 -10.229 1.00 61.94
ATOM 1141 CD LYS A 852 -20.672 8.239 -10.404 1.00 66.23
ATOM 1142 CE LYS A 852 -21.375 7.079 -9.703 1.00 66.46
ATOM 1143 NZ LYS A 852 -22.871 7.181 -9.873 1.00 66.94
ATOM 1144 N SER A 853 -16.671 8.837 -13.145 1.00 62.50
ATOM 1145 CA SER A 853 -16.212 7.989 -14.233 1.00 62.66
ATOM 1146 C SER A 853 -16.012 8.924 -15.431 1.00 61.67
ATOM 1147 O SER A 853 -16.624 9.988 -15.499 1.00 60.83
ATOM 1148 CB SER A 853 -17.233 6.882 -14.536 1.00 63.56
ATOM 1149 OG SER A 853 -18.560 7.374 -14.594 1.00 66.67
ATOM 1150 N PRO A 854 -15.134 8.551 -16.373 1.00 60.36
ATOM 1151 CA PRO A 854 -14.849 9.364 -17.558 1.00 59.12
ATOM 1152 C PRO A 854 -16.065 10.032 -18.179 1.00 57.95
ATOM 1153 O PRO A 854 -16.003 11.182 -18.610 1.00 56.93
ATOM 1154 CB PRO A 854 -14.188 8.365 -18.500 1.00 60.62
ATOM 1155 CG PRO A 854 -13.413 7.508 -17.550 1.00 60.96
ATOM 1156 CD PRO A 854 -14.418 7.263 -16.443 1.00 61.47
ATOM 1157 N ALA A 855 -17.175 9.313 -18.210 1.00 56.59

ATOM 1158 CA ALA A 855 -18.391 9.842 -18.801 1.00 56.60
ATOM 1159 C ALA A 855 -19.414 10.316 -17.762 1.00 55.94
ATOM 1160 O ALA A 855 -20.605 10.376 -18.046 1.00 55.12
ATOM 1161 CB ALA A 855 -19.009 8.779 -19.699 1.00 57.53
ATOM 1162 N HIS A 856 -18.954 10.674 -16.568 1.00 55.98
ATOM 1163 CA HIS A 856 -19.869 11.100 -15.513 1.00 53.27
ATOM 1164 C HIS A 856 -19.169 11.954 -14.460 1.00 51.77
ATOM 1165 O HIS A 856 -18.433 11.446 -13.618 1.00 53.22
ATOM 1166 CB HIS A 856 -20.477 9.858 -14.858 1.00 54.21
ATOM 1167 CG HIS A 856 -21.564 10.146 -13.868 1.00 56.69
ATOM 1168 ND1 HIS A 856 -22.263 9.145 -13.227 1.00 56.79
ATOM 1169 CD2 HIS A 856 -22.080 11.312 -13.416 1.00 55.96
ATOM 1170 CE1 HIS A 856 -23.163 9.681 -12.425 1.00 57.20
ATOM 1171 NE2 HIS A 856 -23.073 10.995 -12.521 1.00 57.31
ATOM 1172 N VAL A 857 -19.397 13.259 -14.514 1.00 49.26
ATOM 1173 CA VAL A 857 -18.794 14.161 -13.550 1.00 46.76
ATOM 1174 C VAL A 857 -19.864 14.686 -12.589 1.00 46.86
ATOM 1175 O VAL A 857 -21.065 14.579 -12.861 1.00 46.96
ATOM 1176 CB VAL A 857 -18.058 15.343 -14.260 1.00 46.02
ATOM 1177 CG1 VAL A 857 -16.777 14.830 -14.928 1.00 41.78
ATOM 1178 CG2 VAL A 857 -18.961 15.992 -15.285 1.00 38.84
ATOM 1179 N LYS A 858 -19.422 15.226 -11.458 1.00 45.57
ATOM 1180 CA LYS A 858 -20.322 15.767 -10.437 1.00 45.68
ATOM 1181 C LYS A 858 -19.765 17.090 -9.923 1.00 45.10
ATOM 1182 O LYS A 858 -18.552 17.220 -9.727 1.00 43.10
ATOM 1183 CB LYS A 858 -20.442 14.804 -9.242 1.00 46.28
ATOM 1184 CG LYS A 858 -21.257 13.521 -9.451 1.00 45.72
ATOM 1185 CD LYS A 858 -21.160 12.646 -8.184 1.00 44.10
ATOM 1186 CE LYS A 858 -21.914 11.324 -8.292 1.00 45.25
ATOM 1187 NZ LYS A 858 -23.401 11.471 -8.255 1.00 47.27
ATOM 1188 N ILE A 859 -20.643 18.068 -9.703 1.00 45.57
ATOM 1189 CA ILE A 859 -20.203 19.363 -9.185 1.00 45.70
ATOM 1190 C ILE A 859 -20.098 19.256 -7.669 1.00 47.41
ATOM 1191 O ILE A 859 -20.981 18.687 -7.023 1.00 48.32
ATOM 1192 CB ILE A 859 -21.185 20.482 -9.547 1.00 44.76
ATOM 1193 CG1 ILE A 859 -21.259 20.622 -11.074 1.00 44.37
ATOM 1194 CG2 ILE A 859 -20.724 21.793 -8.916 1.00 44.21
ATOM 1195 CD1 ILE A 859 -22.156 21.719 -11.561 1.00 40.72
ATOM 1196 N THR A 860 -19.018 19.787 -7.104 1.00 46.98
ATOM 1197 CA THR A 860 -18.811 19.711 -5.662 1.00 47.63
ATOM 1198 C THR A 860 -18.467 21.050 -5.024 1.00 48.69
ATOM 1199 O THR A 860 -18.155 22.019 -5.711 1.00 49.80
ATOM 1200 CB THR A 860 -17.670 18.714 -5.308 1.00 46.89
ATOM 1201 OG1 THR A 860 -17.661 18.468 -3.897 1.00 45.80
ATOM 1202 CG2 THR A 860 -16.322 19.295 -5.686 1.00 44.93

ATOM 1203 N ASP A 861 -18.526 21.078 -3.696 1.00 49.00
ATOM 1204 CA ASP A 861 -18.195 22.253 -2.897 1.00 51.12
ATOM 1205 C ASP A 861 -19.116 23.454 -2.982 1.00 52.18
ATOM 1206 O ASP A 861 -18.722 24.560 -2.630 1.00 53.11
ATOM 1207 CB ASP A 861 -16.767 22.716 -3.177 1.00 49.84
ATOM 1208 CG ASP A 861 -16.057 23.146 -1.914 1.00 52.95
ATOM 1209 OD1 ASP A 861 -16.108 22.375 -0.941 1.00 55.50
ATOM 1210 OD2 ASP A 861 -15.451 24.233 -1.871 1.00 55.17
ATOM 1211 N PHE A 862 -20.340 23.254 -3.440 1.00 54.22
ATOM 1212 CA PHE A 862 -21.269 24.367 -3.500 1.00 57.56
ATOM 1213 C PHE A 862 -21.792 24.637 -2.080 1.00 61.09
ATOM 1214 O PHE A 862 -22.294 23.734 -1.410 1.00 62.23
ATOM 1215 CB PHE A 862 -22.429 24.032 -4.437 1.00 55.96
ATOM 1216 CG PHE A 862 -23.035 22.671 -4.197 1.00 55.99
ATOM 1217 CD1 PHE A 862 -22.751 21.609 -5.051 1.00 56.15
ATOM 1218 CD2 PHE A 862 -23.883 22.448 -3.115 1.00 53.52
ATOM 1219 CE1 PHE A 862 -23.302 20.348 -4.829 1.00 56.04
ATOM 1220 CE2 PHE A 862 -24.435 21.195 -2.886 1.00 52.92
ATOM 1221 CZ PHE A 862 -24.144 20.141 -3.746 1.00 54.63
ATOM 1222 N GLY A 863 -21.651 25.866 -1.600 1.00 64.10
ATOM 1223 CA GLY A 863 -22.153 26.162 -0.268 1.00 67.86
ATOM 1224 C GLY A 863 -21.176 26.776 0.716 1.00 70.52
ATOM 1225 O GLY A 863 -21.529 27.720 1.427 1.00 70.56
ATOM 1226 N LEU A 864 -19.959 26.240 0.780 1.00 72.06
ATOM 1227 CA LEU A 864 -18.953 26.772 1.691 1.00 73.84
ATOM 1228 C LEU A 864 -18.657 28.229 1.337 1.00 75.19
ATOM 1229 O LEU A 864 -18.297 29.027 2.199 1.00 77.44
ATOM 1230 CB LEU A 864 -17.660 25.955 1.610 1.00 73.25
ATOM 1231 CG LEU A 864 -17.786 24.442 1.773 1.00 72.21
ATOM 1232 CD1 LEU A 864 -16.405 23.833 1.808 1.00 71.56
ATOM 1233 CD2 LEU A 864 -18.543 24.115 3.037 1.00 71.95
ATOM 1234 N ALA A 865 -18.812 28.569 0.064 1.00 75.54
ATOM 1235 CA ALA A 865 -18.564 29.924 -0.403 1.00 75.51
ATOM 1236 C ALA A 865 -19.274 30.937 0.485 1.00 76.03
ATOM 1237 O ALA A 865 -18.654 31.859 1.020 1.00 77.18
ATOM 1238 CB ALA A 865 -19.048 30.067 -1.834 1.00 76.59
ATOM 1239 N ARG A 866 -20.579 30.757 0.641 1.00 75.54
ATOM 1240 CA ARG A 866 -21.389 31.661 1.448 1.00 74.65
ATOM 1241 C ARG A 866 -21.168 31.435 2.940 1.00 73.26
ATOM 1242 O ARG A 866 -21.048 32.382 3.716 1.00 72.57
ATOM 1243 CB ARG A 866 -22.869 31.456 1.116 1.00 75.86
ATOM 1244 CG ARG A 866 -23.797 32.543 1.621 1.00 78.29
ATOM 1245 CD ARG A 866 -25.223 32.212 1.231 1.00 81.93
ATOM 1246 NE ARG A 866 -26.098 33.379 1.227 1.00 85.05
ATOM 1247 CZ ARG A 866 -27.359 33.362 0.800 1.00 87.00

```
ATOM   1248  NH1 ARG A 866     -27.893  32.233   0.343  1.00 86.94
ATOM   1249  NH2 ARG A 866     -28.082  34.476   0.816  1.00 88.11
ATOM   1250  N   LEU A 867     -21.104  30.172   3.333  1.00 71.68
ATOM   1251  CA  LEU A 867     -20.929  29.817   4.732  1.00 71.24
ATOM   1252  C   LEU A 867     -19.657  30.365   5.369  1.00 70.68
ATOM   1253  O   LEU A 867     -19.642  30.649   6.566  1.00 70.39
ATOM   1254  CB  LEU A 867     -20.963  28.296   4.885  1.00 70.78
ATOM   1255  CG  LEU A 867     -21.160  27.766   6.300  1.00 69.00
ATOM   1256  CD1 LEU A 867     -22.544  28.150   6.800  1.00 70.14
ATOM   1257  CD2 LEU A 867     -21.006  26.262   6.299  1.00 69.35
ATOM   1258  N   LEU A 868     -18.597  30.519   4.579  1.00 70.51
ATOM   1259  CA  LEU A 868     -17.333  31.021   5.108  1.00 70.64
ATOM   1260  C   LEU A 868     -17.202  32.537   5.032  1.00 71.18
ATOM   1261  O   LEU A 868     -16.786  33.179   5.996  1.00 71.59
ATOM   1262  CB  LEU A 868     -16.152  30.362   4.390  1.00 70.84
ATOM   1263  CG  LEU A 868     -16.175  28.826   4.286  1.00 72.40
ATOM   1264  CD1 LEU A 868     -14.780  28.326   3.889  1.00 70.82
ATOM   1265  CD2 LEU A 868     -16.614  28.201   5.610  1.00 70.35
ATOM   1266  N   GLU A 869     -17.549  33.121   3.894  1.00 72.14
ATOM   1267  CA  GLU A 869     -17.456  34.567   3.771  1.00 72.99
ATOM   1268  C   GLU A 869     -18.658  35.262   4.389  1.00 72.22
ATOM   1269  O   GLU A 869     -18.633  35.645   5.558  1.00 72.77
ATOM   1270  CB  GLU A 869     -17.316  34.968   2.311  1.00 74.69
ATOM   1271  CG  GLU A 869     -15.925  34.742   1.782  1.00 78.22
ATOM   1272  CD  GLU A 869     -15.688  35.427   0.451  1.00 81.09
ATOM   1273  OE1 GLU A 869     -14.505  35.593   0.097  1.00 81.80
ATOM   1274  OE2 GLU A 869     -16.671  35.793  -0.241  1.00 81.14
ATOM   1275  N   GLY A 870     -19.713  35.415   3.602  1.00 71.14
ATOM   1276  CA  GLY A 870     -20.910  36.064   4.093  1.00 69.73
ATOM   1277  C   GLY A 870     -21.585  36.758   2.941  1.00 69.34
ATOM   1278  O   GLY A 870     -21.266  36.488   1.788  1.00 67.87
ATOM   1279  N   ASP A 871     -22.514  37.654   3.245  1.00 70.63
ATOM   1280  CA  ASP A 871     -23.221  38.388   2.206  1.00 71.41
ATOM   1281  C   ASP A 871     -22.979  39.888   2.287  1.00 69.67
ATOM   1282  O   ASP A 871     -23.710  40.673   1.693  1.00 70.04
ATOM   1283  CB  ASP A 871     -24.720  38.092   2.291  1.00 75.78
ATOM   1284  CG  ASP A 871     -25.081  36.742   1.692  1.00 80.13
ATOM   1285  OD1 ASP A 871     -25.017  36.611   0.448  1.00 82.71
ATOM   1286  OD2 ASP A 871     -25.419  35.811   2.458  1.00 81.77
ATOM   1287  N   GLU A 872     -21.945  40.288   3.018  1.00 69.40
ATOM   1288  CA  GLU A 872     -21.638  41.704   3.156  1.00 69.92
ATOM   1289  C   GLU A 872     -21.292  42.261   1.783  1.00 67.97
ATOM   1290  O   GLU A 872     -20.261  41.926   1.204  1.00 67.08
ATOM   1291  CB  GLU A 872     -20.469  41.902   4.125  1.00 72.87
ATOM   1292  CG  GLU A 872     -20.340  43.319   4.675  1.00 78.70
```

```
ATOM   1293  CD  GLU A 872     -19.204  43.458   5.689  1.00 83.05
ATOM   1294  OE1 GLU A 872     -19.079  44.535   6.318  1.00 83.94
ATOM   1295  OE2 GLU A 872     -18.429  42.490   5.857  1.00 86.32
ATOM   1296  N   LYS A 873     -22.169  43.109   1.264  1.00 66.05
ATOM   1297  CA  LYS A 873     -21.976  43.703  -0.046  1.00 65.17
ATOM   1298  C   LYS A 873     -20.551  44.188  -0.314  1.00 64.82
ATOM   1299  O   LYS A 873     -19.998  43.941  -1.380  1.00 64.23
ATOM   1300  CB  LYS A 873     -22.956  44.864  -0.234  1.00 65.59
ATOM   1301  CG  LYS A 873     -22.803  45.611  -1.561  1.00 68.09
ATOM   1302  CD  LYS A 873     -23.875  46.686  -1.729  1.00 69.73
ATOM   1303  CE  LYS A 873     -23.672  47.499  -3.007  1.00 71.60
ATOM   1304  NZ  LYS A 873     -24.749  48.517  -3.211  1.00 71.19
ATOM   1305  N   GLU A 874     -19.949  44.873   0.652  1.00 65.02
ATOM   1306  CA  GLU A 874     -18.603  45.397   0.454  1.00 63.95
ATOM   1307  C   GLU A 874     -17.487  44.565   1.065  1.00 62.00
ATOM   1308  O   GLU A 874     -17.587  44.080   2.194  1.00 62.31
ATOM   1309  CB  GLU A 874     -18.518  46.840   0.964  1.00 65.71
ATOM   1310  CG  GLU A 874     -19.059  47.045   2.363  1.00 69.44
ATOM   1311  CD  GLU A 874     -20.576  46.946   2.437  1.00 71.62
ATOM   1312  OE1 GLU A 874     -21.259  47.887   1.973  1.00 71.73
ATOM   1313  OE2 GLU A 874     -21.083  45.923   2.955  1.00 72.76
ATOM   1314  N   TYR A 875     -16.422  44.399   0.290  1.00 59.06
ATOM   1315  CA  TYR A 875     -15.259  43.641   0.720  1.00 57.62
ATOM   1316  C   TYR A 875     -14.381  44.522   1.587  1.00 57.53
ATOM   1317  O   TYR A 875     -14.266  45.724   1.349  1.00 56.84
ATOM   1318  CB  TYR A 875     -14.414  43.225  -0.480  1.00 56.65
ATOM   1319  CG  TYR A 875     -15.098  42.342  -1.484  1.00 56.70
ATOM   1320  CD1 TYR A 875     -15.421  41.027  -1.173  1.00 56.15
ATOM   1321  CD2 TYR A 875     -15.402  42.817  -2.759  1.00 55.46
ATOM   1322  CE1 TYR A 875     -16.027  40.205  -2.103  1.00 56.63
ATOM   1323  CE2 TYR A 875     -16.007  42.005  -3.697  1.00 55.93
ATOM   1324  CZ  TYR A 875     -16.319  40.697  -3.362  1.00 56.44
ATOM   1325  OH  TYR A 875     -16.933  39.879  -4.275  1.00 55.10
ATOM   1326  N   ASN A 876     -13.760  43.933   2.597  1.00 57.67
ATOM   1327  CA  ASN A 876     -12.852  44.705   3.409  1.00 58.46
ATOM   1328  C   ASN A 876     -11.471  44.340   2.859  1.00 59.52
ATOM   1329  O   ASN A 876     -11.382  43.709   1.806  1.00 58.53
ATOM   1330  CB  ASN A 876     -13.016  44.393   4.908  1.00 59.97
ATOM   1331  CG  ASN A 876     -12.785  42.934   5.255  1.00 63.94
ATOM   1332  OD1 ASN A 876     -11.833  42.311   4.775  1.00 67.34
ATOM   1333  ND2 ASN A 876     -13.642  42.387   6.125  1.00 61.21
ATOM   1334  N   ALA A 877     -10.405  44.736   3.546  1.00 60.79
ATOM   1335  CA  ALA A 877      -9.041  44.483   3.081  1.00 61.10
ATOM   1336  C   ALA A 877      -8.689  43.019   2.829  1.00 62.40
ATOM   1337  O   ALA A 877      -7.782  42.714   2.046  1.00 61.52
```

```
ATOM   1338  CB  ALA A 877     -8.058  45.080   4.066  1.00 60.97
ATOM   1339  N   ASP A 878     -9.409  42.122   3.494  1.00 63.27
ATOM   1340  CA  ASP A 878     -9.172  40.690   3.370  1.00 63.19
ATOM   1341  C   ASP A 878     -9.636  40.145   2.022  1.00 63.64
ATOM   1342  O   ASP A 878     -9.158  39.107   1.569  1.00 63.47
ATOM   1343  CB  ASP A 878     -9.879  39.958   4.509  1.00 62.08
ATOM   1344  CG  ASP A 878     -9.278  38.604   4.787  1.00 64.16
ATOM   1345  OD1 ASP A 878     -8.034  38.520   4.917  1.00 63.46
ATOM   1346  OD2 ASP A 878    -10.047  37.624   4.885  1.00 65.45
ATOM   1347  N   GLY A 879    -10.571  40.848   1.387  1.00 64.96
ATOM   1348  CA  GLY A 879    -11.081  40.422   0.092  1.00 66.39
ATOM   1349  C   GLY A 879    -11.894  39.139   0.105  1.00 66.47
ATOM   1350  O   GLY A 879    -12.483  38.779   1.124  1.00 67.04
ATOM   1351  N   GLY A 880    -11.920  38.443  -1.031  1.00 66.80
ATOM   1352  CA  GLY A 880    -12.676  37.204  -1.127  1.00 66.89
ATOM   1353  C   GLY A 880    -11.850  35.931  -1.217  1.00 66.50
ATOM   1354  O   GLY A 880    -10.679  35.976  -1.586  1.00 67.73
ATOM   1355  N   LYS A 881    -12.461  34.793  -0.892  1.00 66.57
ATOM   1356  CA  LYS A 881    -11.773  33.503  -0.935  1.00 67.51
ATOM   1357  C   LYS A 881    -11.804  32.841  -2.316  1.00 66.54
ATOM   1358  O   LYS A 881    -10.988  31.958  -2.597  1.00 66.96
ATOM   1359  CB  LYS A 881    -12.353  32.538   0.116  1.00 69.38
ATOM   1360  CG  LYS A 881    -12.196  33.032   1.552  1.00 73.80
ATOM   1361  CD  LYS A 881    -12.514  31.966   2.608  1.00 76.95
ATOM   1362  CE  LYS A 881    -12.271  32.525   4.032  1.00 79.84
ATOM   1363  NZ  LYS A 881    -12.387  31.531   5.153  1.00 77.75
ATOM   1364  N   MET A 882    -12.738  33.255  -3.172  1.00 63.86
ATOM   1365  CA  MET A 882    -12.822  32.682  -4.512  1.00 62.87
ATOM   1366  C   MET A 882    -11.752  33.268  -5.420  1.00 59.24
ATOM   1367  O   MET A 882    -11.448  34.453  -5.344  1.00 59.24
ATOM   1368  CB  MET A 882    -14.182  32.957  -5.152  1.00 67.37
ATOM   1369  CG  MET A 882    -15.308  32.094  -4.663  1.00 73.66
ATOM   1370  SD  MET A 882    -15.853  32.567  -3.040  1.00 80.15
ATOM   1371  CE  MET A 882    -15.822  30.977  -2.239  1.00 79.51
ATOM   1372  N   PRO A 883    -11.175  32.447  -6.303  1.00 55.61
ATOM   1373  CA  PRO A 883    -10.150  33.005  -7.180  1.00 54.96
ATOM   1374  C   PRO A 883    -10.749  34.048  -8.127  1.00 54.82
ATOM   1375  O   PRO A 883    -11.750  33.794  -8.788  1.00 54.42
ATOM   1376  CB  PRO A 883     -9.598  31.769  -7.892  1.00 54.93
ATOM   1377  CG  PRO A 883    -10.765  30.818  -7.897  1.00 55.39
ATOM   1378  CD  PRO A 883    -11.367  31.006  -6.539  1.00 54.78
ATOM   1379  N   ILE A 884    -10.122  35.221  -8.166  1.00 55.44
ATOM   1380  CA  ILE A 884    -10.536  36.360  -8.986  1.00 55.16
ATOM   1381  C   ILE A 884    -10.812  36.062 -10.462  1.00 54.77
ATOM   1382  O   ILE A 884    -11.743  36.609 -11.052  1.00 54.35
```

ATOM 1383 CB ILE A 884 -9.457 37.490 -8.930 1.00 57.82
ATOM 1384 CG1 ILE A 884 -9.280 37.996 -7.492 1.00 60.91
ATOM 1385 CG2 ILE A 884 -9.863 38.658 -9.812 1.00 57.84
ATOM 1386 CD1 ILE A 884 -10.456 38.817 -6.963 1.00 61.63
ATOM 1387 N LYS A 885 -10.003 35.196 -11.057 1.00 54.04
ATOM 1388 CA LYS A 885 -10.126 34.878 -12.476 1.00 53.74
ATOM 1389 C LYS A 885 -11.342 34.054 -12.922 1.00 52.87
ATOM 1390 O LYS A 885 -11.586 33.890 -14.117 1.00 53.63
ATOM 1391 CB LYS A 885 -8.823 34.222 -12.937 1.00 55.38
ATOM 1392 CG LYS A 885 -7.609 35.112 -12.690 1.00 57.08
ATOM 1393 CD LYS A 885 -6.308 34.437 -13.069 1.00 59.92
ATOM 1394 CE LYS A 885 -5.131 35.372 -12.845 1.00 62.00
ATOM 1395 NZ LYS A 885 -3.829 34.700 -13.114 1.00 65.60
ATOM 1396 N TRP A 886 -12.108 33.546 -11.967 1.00 50.16
ATOM 1397 CA TRP A 886 -13.304 32.766 -12.271 1.00 47.41
ATOM 1398 C TRP A 886 -14.526 33.578 -11.836 1.00 47.34
ATOM 1399 O TRP A 886 -15.664 33.109 -11.882 1.00 47.47
ATOM 1400 CB TRP A 886 -13.268 31.461 -11.483 1.00 45.53
ATOM 1401 CG TRP A 886 -12.483 30.373 -12.121 1.00 45.12
ATOM 1402 CD1 TRP A 886 -12.967 29.373 -12.911 1.00 42.75
ATOM 1403 CD2 TRP A 886 -11.077 30.149 -12.004 1.00 44.61
ATOM 1404 NE1 TRP A 886 -11.952 28.536 -13.288 1.00 42.27
ATOM 1405 CE2 TRP A 886 -10.778 28.989 -12.747 1.00 43.80
ATOM 1406 CE3 TRP A 886 -10.038 30.814 -11.344 1.00 45.37
ATOM 1407 CZ2 TRP A 886 -9.477 28.476 -12.850 1.00 41.96
ATOM 1408 CZ3 TRP A 886 -8.743 30.302 -11.448 1.00 45.18
ATOM 1409 CH2 TRP A 886 -8.478 29.144 -12.197 1.00 40.59
ATOM 1410 N MET A 887 -14.266 34.809 -11.428 1.00 45.49
ATOM 1411 CA MET A 887 -15.292 35.689 -10.903 1.00 47.92
ATOM 1412 C MET A 887 -15.945 36.606 -11.924 1.00 47.15
ATOM 1413 O MET A 887 -15.286 37.112 -12.826 1.00 46.97
ATOM 1414 CB MET A 887 -14.655 36.521 -9.781 1.00 50.44
ATOM 1415 CG MET A 887 -15.580 37.050 -8.724 1.00 51.18
ATOM 1416 SD MET A 887 -14.641 37.374 -7.213 1.00 53.31
ATOM 1417 CE MET A 887 -14.838 35.821 -6.359 1.00 55.22
ATOM 1418 N ALA A 888 -17.248 36.814 -11.771 1.00 46.65
ATOM 1419 CA ALA A 888 -17.992 37.707 -12.653 1.00 47.77
ATOM 1420 C ALA A 888 -17.620 39.138 -12.281 1.00 48.61
ATOM 1421 O ALA A 888 -17.515 39.483 -11.104 1.00 48.25
ATOM 1422 CB ALA A 888 -19.491 37.497 -12.486 1.00 45.93
ATOM 1423 N LEU A 889 -17.418 39.965 -13.294 1.00 50.52
ATOM 1424 CA LEU A 889 -17.030 41.350 -13.098 1.00 51.06
ATOM 1425 C LEU A 889 -17.751 42.039 -11.953 1.00 52.52
ATOM 1426 O LEU A 889 -17.122 42.682 -11.104 1.00 52.90
ATOM 1427 CB LEU A 889 -17.270 42.121 -14.387 1.00 52.30

ATOM 1428 CG LEU A 889 -16.926 43.607 -14.399 1.00 53.28
ATOM 1429 CD1 LEU A 889 -15.502 43.802 -13.915 1.00 53.95
ATOM 1430 CD2 LEU A 889 -17.114 44.154 -15.816 1.00 49.72
ATOM 1431 N GLU A 890 -19.072 41.894 -11.919 1.00 52.25
ATOM 1432 CA GLU A 890 -19.864 42.538 -10.881 1.00 52.51
ATOM 1433 C GLU A 890 -19.517 42.070 -9.482 1.00 54.25
ATOM 1434 O GLU A 890 -19.668 42.821 -8.520 1.00 55.68
ATOM 1435 CB GLU A 890 -21.361 42.322 -11.116 1.00 51.54
ATOM 1436 CG GLU A 890 -21.799 40,871 -11.075 1.00 49.82
ATOM 1437 CD GLU A 890 -21.820 40.236 -12.448 1.00 47.38
ATOM 1438 OE1 GLU A 890 -20.989 40.647 -13.299 1.00 40.49
ATOM 1439 OE2 GLU A 890 -22.664 39.326 -12.650 1.00 42.65
ATOM 1440 N CYS A 891 -19.059 40.832 -9.361 1.00 55.67
ATOM 1441 CA CYS A 891 -18.720 40.296 -8.052 1.00 56.74
ATOM 1442 C CYS A 891 -17.300 40.649 -7.605 1.00 57.48
ATOM 1443 O CYS A 891 -16.868 40.297 -6.508 1.00 55.50
ATOM 1444 CB CYS A 891 -18.956 38.781 -8.036 1.00 57.62
ATOM 1445 SG CYS A 891 -20.729 38.333 -7.970 1.00 57.17
ATOM 1446 N ILE A 892 -16.576 41.362 -8.458 1.00 58.80
ATOM 1447 CA ILE A 892 -15.224 41.780 -8.112 1.00 59.01
ATOM 1448 C ILE A 892 -15.285 43.087 -7.319 1.00 59.18
ATOM 1449 O ILE A 892 -14.529 43.274 -6.374 1.00 60.68
ATOM 1450 CB ILE A 892 -14.357 42.018 -9.369 1.00 57.56
ATOM 1451 CG1 ILE A 892 -14.003 40.684 -10.024 1.00 56.20
ATOM 1452 CG2 ILE A 892 -13.104 42.792 -8.996 1.00 54.39
ATOM 1453 CD1 ILE A 892 -13.252 40.841 -11.323 1.00 56.41
ATOM 1454 N HIS A 893 -16.193 43.981 -7.707 1.00 58.73
ATOM 1455 CA HIS A 893 -16.333 45.274 -7.046 1.00 57.13
ATOM 1456 C HIS A 893 -17.139 45.236 -5.757 1.00 55.23
ATOM 1457 O HIS A 893 -16.951 46.075 -4.879 1.00 55.68
ATOM 1458 CB HIS A 893 -16.947 46.276 -8.015 1.00 58.88
ATOM 1459 CG HIS A 893 -16.103 46.532 -9.225 1.00 62.09
ATOM 1460 ND1 HIS A 893 -16.555 46.318 -10.510 1.00 62.92
ATOM 1461 CD2 HIS A 893 -14.825 46.969 -9.344 1.00 63.01
ATOM 1462 CE1 HIS A 893 -15.593 46.609 -11.368 1.00 63.20
ATOM 1463 NE2 HIS A 893 -14.532 47.006 -10.687 1.00 63.80
ATOM 1464 N TYR A 894 -18.031 44.258 -5.652 1.00 53.00
ATOM 1465 CA TYR A 894 -18.887 44.072 -4.477 1.00 51.14
ATOM 1466 C TYR A 894 -19.364 42.639 -4.549 1.00 49.31
ATOM 1467 O TYR A 894 -19.093 41.949 -5.518 1.00 50.31
ATOM 1468 CB TYR A 894 -20.135 44.959 -4.542 1.00 52.50
ATOM 1469 CG TYR A 894 -19.895 46.444 -4.526 1.00 53.58
ATOM 1470 CD1 TYR A 894 -19.719 47.126 -3.327 1.00 54.62
ATOM 1471 CD2 TYR A 894 -19.832 47.167 -5.716 1.00 52.84
ATOM 1472 CE1 TYR A 894 -19.483 48.491 -3.313 1.00 57.08

```
ATOM   1473  CE2 TYR A 894     -19.594  48.529  -5.718  1.00 54.76
ATOM   1474  CZ  TYR A 894     -19.417  49.190  -4.515  1.00 57.74
ATOM   1475  OH  TYR A 894     -19.147  50.546  -4.505  1.00 59.64
ATOM   1476  N   ARG A 895     -20.087  42.195  -3.534  1.00 48.76
ATOM   1477  CA  ARG A 895     -20.624  40.845  -3.535  1.00 50.39
ATOM   1478  C   ARG A 895     -22.022  40.867  -4.152  1.00 50.91
ATOM   1479  O   ARG A 895     -23.002  41.194  -3.486  1.00 51.94
ATOM   1480  CB  ARG A 895     -20.712  40.281  -2.112  1.00 49.62
ATOM   1481  CG  ARG A 895     -19.382  39.914  -1.498  1.00 49.55
ATOM   1482  CD  ARG A 895     -19.526  38.808  -0.460  1.00 49.12
ATOM   1483  NE  ARG A 895     -18.216  38.395   0.034  1.00 53.76
ATOM   1484  CZ  ARG A 895     -17.475  39.124   0.866  1.00 56.50
ATOM   1485  NH1 ARG A 895     -16.284  38.688   1.268  1.00 52.02
ATOM   1486  NH2 ARG A 895     -17.940  40.288   1.316  1.00 57.79
ATOM   1487  N   ALA A 896     -22.109  40.534  -5.432  1.00 51.10
ATOM   1488  CA  ALA A 896     -23.392  40.505  -6.122  1.00 49.65
ATOM   1489  C   ALA A 896     -23.571  39.101  -6.670  1.00 47.43
ATOM   1490  O   ALA A 896     -23.849  38.925  -7.843  1.00 46.98
ATOM   1491  CB  ALA A 896     -23.405  41.530  -7.266  1.00 49.62
ATOM   1492  N   PHE A 897     -23.417  38.098  -5.816  1.00 46.40
ATOM   1493  CA  PHE A 897     -23.540  36.721  -6.276  1.00 46.89
ATOM   1494  C   PHE A 897     -24.943  36.276  -6.689  1.00 45.30
ATOM   1495  O   PHE A 897     -25.889  36.296  -5.902  1.00 44.45
ATOM   1496  CB  PHE A 897     -22.965  35.759  -5.231  1.00 47.33
ATOM   1497  CG  PHE A 897     -21.487  35.887  -5.058  1.00 48.54
ATOM   1498  CD1 PHE A 897     -20.952  36.469  -3.909  1.00 51.22
ATOM   1499  CD2 PHE A 897     -20.622  35.458  -6.061  1.00 49.59
ATOM   1500  CE1 PHE A 897     -19.567  36.627  -3.764  1.00 50.13
ATOM   1501  CE2 PHE A 897     -19.239  35.607  -5.932  1.00 49.10
ATOM   1502  CZ  PHE A 897     -18.709  36.194  -4.780  1.00 50.78
ATOM   1503  N   THR A 898     -25.055  35.867  -7.946  1.00 44.73
ATOM   1504  CA  THR A 898     -26.324  35.413  -8.499  1.00 44.26
ATOM   1505  C   THR A 898     -26.085  34.245  -9.422  1.00 43.33
ATOM   1506  O   THR A 898     -24.942  33.943  -9.774  1.00 42.13
ATOM   1507  CB  THR A 898     -27.000  36.497  -9.356  1.00 44.01
ATOM   1508  OG1 THR A 898     -26.211  36.730 -10.529  1.00 43.71
ATOM   1509  CG2 THR A 898     -27.148  37.786  -8.571  1.00 44.17
ATOM   1510  N   HIS A 899     -27.171  33.595  -9.821  1.00 41.98
ATOM   1511  CA  HIS A 899     -27.065  32.487 -10.748  1.00 42.31
ATOM   1512  C   HIS A 899     -26.317  32.987 -11.982  1.00 41.21
ATOM   1513  O   HIS A 899     -25.520  32.255 -12.567  1.00 42.33
ATOM   1514  CB  HIS A 899     -28.457  31.985 -11.113  1.00 43.29
ATOM   1515  CG  HIS A 899     -29.246  31.542  -9.927  1.00 45.33
ATOM   1516  ND1 HIS A 899     -28.795  30.571  -9.057  1.00 47.28
ATOM   1517  CD2 HIS A 899     -30.433  31.968  -9.435  1.00 46.03
```

ATOM 1518 CE1 HIS A 899 -29.667 30.418 -8.078 1.00 46.75
ATOM 1519 NE2 HIS A 899 -30.670 31.255 -8.283 1.00 49.17
ATOM 1520 N GLN A 900 -26.540 34.243 -12.358 1.00 39.59
ATOM 1521 CA GLN A 900 -25.842 34.776 -13.521 1.00 40.74
ATOM 1522 C GLN A 900 -24.325 34.960 -13.315 1.00 39.29
ATOM 1523 O GLN A 900 -23.565 34.901 -14.276 1.00 37.94
ATOM 1524 CB GLN A 900 -26.497 36.078 -14.002 1.00 40.33
ATOM 1525 CG GLN A 900 -27.937 35.893 -14.495 1.00 44.02
ATOM 1526 CD GLN A 900 -28.125 34.695 -15.443 1.00 47.54
ATOM 1527 OE1 GLN A 900 -28.722 33.677 -15.084 1.00 51.69
ATOM 1528 NE2 GLN A 900 -27.610 34.822 -16.660 1.00 48.77
ATOM 1529 N SER A 901 -23.869 35.171 -12.084 1.00 38.33
ATOM 1530 CA SER A 901 -22.428 35.303 -11.870 1.00 37.53
ATOM 1531 C SER A 901 -21.856 33.895 -12.004 1.00 40.00
ATOM 1532 O SER A 901 -20.757 33.702 -12.542 1.00 39.46
ATOM 1533 CB SER A 901 -22.116 35.891 -10.492 1.00 36.74
ATOM 1534 OG SER A 901 -22.775 35.195 -9.451 1.00 40.58
ATOM 1535 N ASP A 902 -22.626 32.913 -11.527 1.00 39.02
ATOM 1536 CA ASP A 902 -22.247 31.511 -11.623 1.00 37.25
ATOM 1537 C ASP A 902 -22.061 31.163 -13.110 1.00 37.82
ATOM 1538 O ASP A 902 -21.139 30.436 -13.480 1.00 37.20
ATOM 1539 CB ASP A 902 -23.337 30.624 -11.005 1.00 38.66
ATOM 1540 CG ASP A 902 -23.065 30.279 -9.533 1.00 40.83
ATOM 1541 OD1 ASP A 902 -22.241 30.958 -8.896 1.00 41.45
ATOM 1542 OD2 ASP A 902 -23.682 29.326 -9.004 1.00 42.94
ATOM 1543 N VAL A 903 -22.929 31.694 -13.966 1.00 36.71
ATOM 1544 CA VAL A 903 -22.819 31.414 -15.390 1.00 37.25
ATOM 1545 C VAL A 903 -21.473 31.890 -15.932 1.00 37.89
ATOM 1546 O VAL A 903 -20.866 31.234 -16.788 1.00 35.97
ATOM 1547 CB VAL A 903 -23.960 32.075 -16.191 1.00 37.16
ATOM 1548 CG1 VAL A 903 -23.578 32.159 -17.657 1.00 35.90
ATOM 1549 CG2 VAL A 903 -25.232 31.264 -16.043 1.00 34.45
ATOM 1550 N TRP A 904 -21.013 33.035 -15.435 1.00 38.74
ATOM 1551 CA TRP A 904 -19.722 33.574 -15.845 1.00 37.48
ATOM 1552 C TRP A 904 -18.660 32.523 -15.494 1.00 35.96
ATOM 1553 O TRP A 904 -17.845 32.134 -16.323 1.00 33.79
ATOM 1554 CB TRP A 904 -19.426 34.875 -15.084 1.00 39.00
ATOM 1555 CG TRP A 904 -18.094 35.469 -15.435 1.00 41.83
ATOM 1556 CD1 TRP A 904 -16.870 34.876 -15.304 1.00 40.23
ATOM 1557 CD2 TRP A 904 -17.858 36.746 -16.041 1.00 43.43
ATOM 1558 NE1 TRP A 904 -15.891 35.695 -15.799 1.00 41.66
ATOM 1559 CE2 TRP A 904 -16.464 36.853 -16.255 1.00 44.01
ATOM 1560 CE3 TRP A 904 -18.688 37.810 -16.425 1.00 44.89
ATOM 1561 CZ2 TRP A 904 -15.876 37.989 -16.840 1.00 45.74
ATOM 1562 CZ3 TRP A 904 -18.105 38.943 -17.010 1.00 46.53

```
ATOM   1563  CH2 TRP A 904     -16.710  39.020 -17.210  1.00 46.91
ATOM   1564  N   SER A 905     -18.681  32.070 -14.249  1.00 34.90
ATOM   1565  CA  SER A 905     -17.731  31.078 -13.794  1.00 38.24
ATOM   1566  C   SER A 905     -17.793  29.865 -14.726  1.00 38.83
ATOM   1567  O   SER A 905     -16.773  29.409 -15.250  1.00 41.08
ATOM   1568  CB  SER A 905     -18.059  30.690 -12.354  1.00 39.02
ATOM   1569  OG  SER A 905     -18.186  31.852 -11.545  1.00 39.18
ATOM   1570  N   TYR A 906     -19.000  29.361 -14.935  1.00 38.14
ATOM   1571  CA  TYR A 906     -19.231  28.233 -15.825  1.00 36.99
ATOM   1572  C   TYR A 906     -18.456  28.460 -17.123  1.00 37.89
ATOM   1573  O   TYR A 906     -17.770  27.574 -17.620  1.00 37.22
ATOM   1574  CB  TYR A 906     -20.727  28.127 -16.130  1.00 37.09
ATOM   1575  CG  TYR A 906     -21.060  27.090 -17.169  1.00 36.26
ATOM   1576  CD1 TYR A 906     -21.299  25.767 -16.809  1.00 33.65
ATOM   1577  CD2 TYR A 906     -21.056  27.421 -18.522  1.00 35.93
ATOM   1578  CE1 TYR A 906     -21.513  24.800 -17.765  1.00 35.24
ATOM   1579  CE2 TYR A 906     -21.269  26.461 -19.488  1.00 36.62
ATOM   1580  CZ  TYR A 906     -21.494  25.147 -19.108  1.00 35.06
ATOM   1581  OH  TYR A 906     -21.659  24.187 -20.077  1.00 32.16
ATOM   1582  N   GLY A 907     -18.585  29.658 -17.677  1.00 38.18
ATOM   1583  CA  GLY A 907     -17.866  29.974 -18.890  1.00 37.34
ATOM   1584  C   GLY A 907     -16.368  29.758 -18.734  1.00 39.60
ATOM   1585  O   GLY A 907     -15.749  29.097 -19.583  1.00 39.30
ATOM   1586  N   VAL A 908     -15.775  30.294 -17.662  1.00 38.75
ATOM   1587  CA  VAL A 908     -14.329  30.144 -17.460  1.00 37.84
ATOM   1588  C   VAL A 908     -14.006  28.678 -17.254  1.00 38.99
ATOM   1589  O   VAL A 908     -12.948  28.189 -17.669  1.00 38.75
ATOM   1590  CB  VAL A 908     -13.810  30.938 -16.233  1.00 38.62
ATOM   1591  CG1 VAL A 908     -12.282  30.912 -16.209  1.00 35.04
ATOM   1592  CG2 VAL A 908     -14.315  32.372 -16.274  1.00 33.97
ATOM   1593  N   THR A 909     -14.939  27.974 -16.627  1.00 38.38
ATOM   1594  CA  THR A 909     -14.764  26.552 -16.375  1.00 37.41
ATOM   1595  C   THR A 909     -14.710  25.688 -17.629  1.00 37.98
ATOM   1596  O   THR A 909     -13.837  24.837 -17.747  1.00 39.71
ATOM   1597  CB  THR A 909     -15.861  26.011 -15.472  1.00 34.91
ATOM   1598  OG1 THR A 909     -15.866  26.753 -14.253  1.00 33.91
ATOM   1599  CG2 THR A 909     -15.610  24.541 -15.161  1.00 34.30
ATOM   1600  N   ILE A 910     -15.629  25.877 -18.569  1.00 38.77
ATOM   1601  CA  ILE A 910     -15.566  25.043 -19.765  1.00 41.06
ATOM   1602  C   ILE A 910     -14.357  25.445 -20.598  1.00 42.01
ATOM   1603  O   ILE A 910     -13.887  24.676 -21.444  1.00 39.07
ATOM   1604  CB  ILE A 910     -16.841  25.128 -20.628  1.00 40.40
ATOM   1605  CG1 ILE A 910     -17.064  26.549 -21.124  1.00 42.79
ATOM   1606  CG2 ILE A 910     -18.022  24.642 -19.822  1.00 43.12
ATOM   1607  CD1 ILE A 910     -18.166  26.673 -22.162  1.00 43.99
```

ATOM 1608 N TRP A 911 -13.857 26.656 -20.347 1.00 42.81
ATOM 1609 CA TRP A 911 -12.689 27.146 -21.052 1.00 43.02
ATOM 1610 C TRP A 911 -11.482 26.324 -20.573 1.00 44.92
ATOM 1611 O TRP A 911 -10.651 25.916 -21.384 1.00 45.96
ATOM 1612 CB TRP A 911 -12.481 28.625 -20.759 1.00 45.39
ATOM 1613 CG TRP A 911 -11.281 29.215 -21.435 1.00 49.15
ATOM 1614 CD1 TRP A 911 -11.238 29.822 -22.660 1.00 50.73
ATOM 1615 CD2 TRP A 911 -9.940 29.249 -20.924 1.00 50.38
ATOM 1616 NE1 TRP A 911 -9.954 30.237 -22.942 1.00 49.91
ATOM 1617 CE2 TRP A 911 -9.138 29.897 -21.892 1.00 51.44
ATOM 1618 CE3 TRP A 911 -9.339 28.794 -19.742 1.00 49.30
ATOM 1619 CZ2 TRP A 911 -7.763 30.101 -21.712 1.00 48.85
ATOM 1620 CZ3 TRP A 911 -7.973 28.997 -19.565 1.00 49.14
ATOM 1621 CH2 TRP A 911 -7.203 29.646 -20.548 1.00 48.84
ATOM 1622 N GLU A 912 -11.388 26.066 -19.268 1.00 44.35
ATOM 1623 CA GLU A 912 -10.277 25.273 -18.755 1.00 45.12
ATOM 1624 C GLU A 912 -10.299 23.922 -19.468 1.00 46.73
ATOM 1625 O GLU A 912 -9.254 23.400 -19.879 1.00 46.06
ATOM 1626 CB GLU A 912 -10.404 25.030 -17.247 1.00 44.17
ATOM 1627 CG GLU A 912 -10.530 26.265 -16.378 1.00 45.56
ATOM 1628 CD GLU A 912 -10.733 25.919 -14.899 1.00 47.51
ATOM 1629 OE1 GLU A 912 -9.766 25.474 -14.243 1.00 48.20
ATOM 1630 OE2 GLU A 912 -11.866 26.080 -14.389 1.00 46.43
ATOM 1631 N LEU A 913 -11.502 23.371 -19.622 1.00 46.87
ATOM 1632 CA LEU A 913 -11.691 22.072 -20.270 1.00 45.49
ATOM 1633 C LEU A 913 -11.261 22.067 -21.724 1.00 46.82
ATOM 1634 O LEU A 913 -10.522 21.179 -22.150 1.00 48.03
ATOM 1635 CB LEU A 913 -13.153 21.643 -20.170 1.00 43.18
ATOM 1636 CG LEU A 913 -13.750 21.713 -18.764 1.00 43.01
ATOM 1637 CD1 LEU A 913 -15.174 21.210 -18.804 1.00 43.13
ATOM 1638 CD2 LEU A 913 -12.916 20.880 -17.790 1.00 40.71
ATOM 1639 N MET A 914 -11.726 23.052 -22.487 1.00 48.63
ATOM 1640 CA MET A 914 -11.374 23.148 -23.903 1.00 50.01
ATOM 1641 C MET A 914 -9.874 23.324 -24.112 1.00 50.22
ATOM 1642 O MET A 914 -9.363 23.007 -25.182 1.00 50.31
ATOM 1643 CB MET A 914 -12.108 24.309 -24.576 1.00 51.66
ATOM 1644 CG MET A 914 -13.611 24.142 -24.660 1.00 54.12
ATOM 1645 SD MET A 914 -14.103 22.502 -25.184 1.00 55.78
ATOM 1646 CE MET A 914 -15.162 22.056 -23.847 1.00 54.82
ATOM 1647 N THR A 915 -9.171 23.846 -23.108 1.00 49.71
ATOM 1648 CA THR A 915 -7.727 24.013 -23.230 1.00 49.12
ATOM 1649 C THR A 915 -7.024 22.881 -22.487 1.00 50.59
ATOM 1650 O THR A 915 -5.851 22.985 -22.133 1.00 50.68
ATOM 1651 CB THR A 915 -7.240 25.361 -22.663 1.00 47.98
ATOM 1652 OG1 THR A 915 -7.532 25.426 -21.260 1.00 49.13

ATOM 1653 CG2 THR A 915 -7.912 26.526 -23.392 1.00 45.99
ATOM 1654 N PHE A 916 -7.756 21.797 -22.250 1.00 51.37
ATOM 1655 CA PHE A 916 -7.208 20.632 -21.571 1.00 51.95
ATOM 1656 C PHE A 916 -6.429 21.033 -20.317 1.00 53.29
ATOM 1657 O PHE A 916 -5.255 20.692 -20.160 1.00 54.44
ATOM 1658 CB PHE A 916 -6.299 19.861 -22.538 1.00 51.51
ATOM 1659 CG PHE A 916 -7.028 19.251 -23.718 1.00 50.02
ATOM 1660 CD1 PHE A 916 -7.835 18.124 -23.555 1.00 50.49
ATOM 1661 CD2 PHE A 916 -6.896 19.792 -24.988 1.00 47.97
ATOM 1662 CE1 PHE A 916 -8.493 17.548 -24.641 1.00 49.30
ATOM 1663 CE2 PHE A 916 -7.548 19.225 -26.073 1.00 49.17
ATOM 1664 CZ PHE A 916 -8.347 18.102 -25.902 1.00 49.74
ATOM 1665 N GLY A 917 -7.090 21.774 -19.433 1.00 54.12
ATOM 1666 CA GLY A 917 -6.455 22.207 -18.204 1.00 53.22
ATOM 1667 C GLY A 917 -5.687 23.516 -18.292 1.00 53.97
ATOM 1668 O GLY A 917 -4.769 23.745 -17.503 1.00 56.50
ATOM 1669 N GLY A 918 -6.046 24.385 -19.229 1.00 51.72
ATOM 1670 CA GLY A 918 -5.339 25.647 -19.336 1.00 52.43
ATOM 1671 C GLY A 918 -5.579 26.544 -18.135 1.00 54.51
ATOM 1672 O GLY A 918 -6.514 26.323 -17.366 1.00 55.43
ATOM 1673 N LYS A 919 -4.742 27.561 -17.964 1.00 55.17
ATOM 1674 CA LYS A 919 -4.902 28.472 -16.838 1.00 55.34
ATOM 1675 C LYS A 919 -5.396 29.852 -17.268 1.00 55.34
ATOM 1676 O LYS A 919 -4.765 30.528 -18.082 1.00 54.75
ATOM 1677 CB LYS A 919 -3.584 28.608 -16.082 1.00 57.86
ATOM 1678 CG LYS A 919 -3.045 27.296 -15.545 1.00 61.37
ATOM 1679 CD LYS A 919 -1.874 27.539 -14.608 1.00 65.00
ATOM 1680 CE LYS A 919 -2.319 28.318 -13.372 1.00 68.24
ATOM 1681 NZ LYS A 919 -1.174 28.718 -12.493 1.00 70.07
ATOM 1682 N PRO A 920 -6.539 30.287 -16.714 1.00 54.70
ATOM 1683 CA PRO A 920 -7.199 31.571 -16.977 1.00 54.08
ATOM 1684 C PRO A 920 -6.248 32.746 -16.833 1.00 53.70
ATOM 1685 O PRO A 920 -5.558 32.860 -15.828 1.00 54.60
ATOM 1686 CB PRO A 920 -8.292 31.617 -15.920 1.00 53.99
ATOM 1687 CG PRO A 920 -8.618 30.190 -15.718 1.00 56.24
ATOM 1688 CD PRO A 920 -7.269 29.535 -15.683 1.00 54.76
ATOM 1689 N TYR A 921 -6.232 33.624 -17.828 1.00 53.96
ATOM 1690 CA TYR A 921 -5.362 34.794 -17.810 1.00 56.43
ATOM 1691 C TYR A 921 -3.992 34.423 -17.242 1.00 59.51
ATOM 1692 O TYR A 921 -3.519 35.029 -16.276 1.00 59.77
ATOM 1693 CB TYR A 921 -5.996 35.904 -16.972 1.00 53.93
ATOM 1694 CG TYR A 921 -7.477 36.069 -17.217 1.00 50.28
ATOM 1695 CD1 TYR A 921 -8.406 35.456 -16.386 1.00 48.21
ATOM 1696 CD2 TYR A 921 -7.947 36.839 -18.281 1.00 47.29
ATOM 1697 CE1 TYR A 921 -9.760 35.604 -16.597 1.00 47.95

ATOM 1698 CE2 TYR A 921 -9.301 36.993 -18.503 1.00 46.64
ATOM 1699 CZ TYR A 921 -10.204 36.373 -17.654 1.00 48.17
ATOM 1700 OH TYR A 921 -11.552 36.534 -17.841 1.00 46.47
ATOM 1701 N ASP A 922 -3.369 33.424 -17.859 1.00 62.28
ATOM 1702 CA ASP A 922 -2.070 32.918 -17.437 1.00 65.68
ATOM 1703 C ASP A 922 -0.996 33.989 -17.291 1.00 67.52
ATOM 1704 O ASP A 922 -0.560 34.580 -18.281 1.00 68.07
ATOM 1705 CB ASP A 922 -1.573 31.869 -18.427 1.00 66.85
ATOM 1706 CG ASP A 922 -0.510 30.977 -17.830 1.00 69.00
ATOM 1707 OD1 ASP A 922 0.262 31.468 -16.972 1.00 68.93
ATOM 1708 OD2 ASP A 922 -0.445 29.790 -18.223 1.00 69.13
ATOM 1709 N GLY A 923 -0.564 34.221 -16.055 1.00 69.33
ATOM 1710 CA GLY A 923 0.468 35.212 -15.800 1.00 70.77
ATOM 1711 C GLY A 923 -0.022 36.553 -15.281 1.00 71.67
ATOM 1712 O GLY A 923 0.477 37.054 -14.270 1.00 72.97
ATOM 1713 N ILE A 924 -0.995 37.135 -15.973 1.00 71.05
ATOM 1714 CA ILE A 924 -1.548 38.428 -15.592 1.00 70.63
ATOM 1715 C ILE A 924 -1.781 38.545 -14.082 1.00 70.88
ATOM 1716 O ILE A 924 -2.336 37.640 -13.457 1.00 71.74
ATOM 1717 CB ILE A 924 -2.868 38.690 -16.349 1.00 70.59
ATOM 1718 CG1 ILE A 924 -2.652 38.433 -17.848 1.00 70.80
ATOM 1719 CG2 ILE A 924 -3.328 40.127 -16.124 1.00 68.25
ATOM 1720 CD1 ILE A 924 -3.930 38.442 -18.696 1.00 72.84
ATOM 1721 N PRO A 925 -1.340 39.668 -13.480 1.00 70.93
ATOM 1722 CA PRO A 925 -1.446 40.010 -12.055 1.00 70.60
ATOM 1723 C PRO A 925 -2.884 40.065 -11.539 1.00 69.81
ATOM 1724 O PRO A 925 -3.655 40.937 -11.933 1.00 67.59
ATOM 1725 CB PRO A 925 -0.779 41.384 -11.980 1.00 71.26
ATOM 1726 CG PRO A 925 0.207 41.347 -13.091 1.00 70.82
ATOM 1727 CD PRO A 925 -0.599 40.721 -14.196 1.00 70.92
ATOM 1728 N THR A 926 -3.221 39.149 -10.638 1.00 69.20
ATOM 1729 CA THR A 926 -4.559 39.071 -10.061 1.00 70.01
ATOM 1730 C THR A 926 -5.184 40.429 -9.730 1.00 70.43
ATOM 1731 O THR A 926 -6.407 40.578 -9.735 1.00 69.78
ATOM 1732 CB THR A 926 -4.553 38.213 -8.770 1.00 70.42
ATOM 1733 OG1 THR A 926 -5.899 37.915 -8.390 1.00 71.23
ATOM 1734 CG2 THR A 926 -3.870 38.962 -7.623 1.00 71.38
ATOM 1735 N ALA A 927 -4.344 41.417 -9.441 1.00 71.00
ATOM 1736 CA ALA A 927 -4.830 42.746 -9.095 1.00 70.88
ATOM 1737 C ALA A 927 -5.223 43.542 -10.336 1.00 71.19
ATOM 1738 O ALA A 927 -5.820 44.615 -10.237 1.00 72.20
ATOM 1739 CB ALA A 927 -3.759 43.498 -8.305 1.00 69.23
ATOM 1740 N GLU A 928 -4.908 43.008 -11.507 1.00 71.41
ATOM 1741 CA GLU A 928 -5.209 43.709 -12.747 1.00 71.50
ATOM 1742 C GLU A 928 -6.429 43.196 -13.494 1.00 68.69

ATOM 1743 O GLU A 928 -6.968 43.892 -14.355 1.00 68.39
ATOM 1744 CB GLU A 928 -3.983 43.669 -13.659 1.00 73.75
ATOM 1745 CG GLU A 928 -2.754 44.252 -12.996 1.00 78.75
ATOM 1746 CD GLU A 928 -1.535 44.234 -13.891 1.00 82.92
ATOM 1747 OE1 GLU A 928 -0.439 44.579 -13.390 1.00 85.58
ATOM 1748 OE2 GLU A 928 -1.672 43.880 -15.087 1.00 83.54
ATOM 1749 N ILE A 929 -6.868 41.988 -13.167 1.00 65.54
ATOM 1750 CA ILE A 929 -8.027 41.414 -13.831 1.00 63.43
ATOM 1751 C ILE A 929 -9.198 42.407 -13.900 1.00 62.00
ATOM 1752 O ILE A 929 -9.742 42.666 -14.973 1.00 58.78
ATOM 1753 CB ILE A 929 -8.482 40.126 -13.119 1.00 61.81
ATOM 1754 CG1 ILE A 929 -7.336 39.111 -13.105 1.00 61.74
ATOM 1755 CG2 ILE A 929 -9.689 39.538 -13.822 1.00 62.66
ATOM 1756 CD1 ILE A 929 -6.847 38.691 -14.478 1.00 59.86
ATOM 1757 N PRO A 930 -9.584 42.991 -12.755 1.00 61.97
ATOM 1758 CA PRO A 930 -10.694 43.948 -12.732 1.00 62.93
ATOM 1759 C PRO A 930 -10.643 44.976 -13.856 1.00 64.06
ATOM 1760 O PRO A 930 -11.641 45.216 -14.538 1.00 62.58
ATOM 1761 CB PRO A 930 -10.560 44.593 -11.358 1.00 61.80
ATOM 1762 CG PRO A 930 -10.047 43.479 -10.536 1.00 61.59
ATOM 1763 CD PRO A 930 -8.984 42.865 -11.417 1.00 60.70
ATOM 1764 N ASP A 931 -9.476 45.580 -14.046 1.00 66.03
ATOM 1765 CA ASP A 931 -9.311 46.589 -15.081 1.00 68.58
ATOM 1766 C ASP A 931 -9.354 46.006 -16.482 1.00 67.95
ATOM 1767 O ASP A 931 -10.012 46.563 -17.360 1.00 67.90
ATOM 1768 CB ASP A 931 -8.007 47.353 -14.866 1.00 73.60
ATOM 1769 CG ASP A 931 -8.015 48.146 -13.572 1.00 78.41
ATOM 1770 OD1 ASP A 931 -8.154 47.523 -12.485 1.00 79.78
ATOM 1771 OD2 ASP A 931 -7.890 49.391 -13.645 1.00 80.42
ATOM 1772 N LEU A 932 -8.654 44.896 -16.698 1.00 67.05
ATOM 1773 CA LEU A 932 -8.660 44.252 -18.007 1.00 66.68
ATOM 1774 C LEU A 932 -10.110 44.019 -18.434 1.00 67.26
ATOM 1775 O LEU A 932 -10.551 44.492 -19.484 1.00 67.71
ATOM 1776 CB LEU A 932 -7.932 42.909 -17.946 1.00 66.91
ATOM 1777 CG LEU A 932 -6.415 42.931 -17.754 1.00 68.66
ATOM 1778 CD1 LEU A 932 -5.905 41.504 -17.553 1.00 67.81
ATOM 1779 CD2 LEU A 932 -5.753 43.581 -18.977 1.00 68.04
ATOM 1780 N LEU A 933 -10.849 43.297 -17.599 1.00 66.10
ATOM 1781 CA LEU A 933 -12.240 42.982 -17.874 1.00 65.55
ATOM 1782 C LEU A 933 -13.049 44.190 -18.319 1.00 65.37
ATOM 1783 O LEU A 933 -13.751 44.135 -19.331 1.00 65.79
ATOM 1784 CB LEU A 933 -12.878 42.355 -16.638 1.00 64.86
ATOM 1785 CG LEU A 933 -12.233 41.030 -16.223 1.00 65.13
ATOM 1786 CD1 LEU A 933 -12.696 40.652 -14.828 1.00 65.75
ATOM 1787 CD2 LEU A 933 -12.579 39.945 -17.229 1.00 63.48

ATOM 1788 N GLU A 934 -12.947 45.280 -17.567 1.00 65.40
ATOM 1789 CA GLU A 934 -13.687 46.497 -17.885 1.00 65.09
ATOM 1790 C GLU A 934 -13.162 47.174 -19.132 1.00 63.61
ATOM 1791 O GLU A 934 -13.890 47.907 -19.797 1.00 61.44
ATOM 1792 CB GLU A 934 -13.657 47.451 -16.693 1.00 65.83
ATOM 1793 CG GLU A 934 -14.514 46.926 -15.558 1.00 71.06
ATOM 1794 CD GLU A 934 -14.315 47.656 -14.251 1.00 73.66
ATOM 1795 OE1 GLU A 934 -13.217 47.534 -13.659 1.00 75.01
ATOM 1796 OE2 GLU A 934 -15.267 48.344 -13.815 1.00 75.23
ATOM 1797 N LYS A 935 -11.896 46.926 -19.446 1.00 63.09
ATOM 1798 CA LYS A 935 -11.305 47.492 -20.644 1.00 64.10
ATOM 1799 C LYS A 935 -11.907 46.696 -21.792 1.00 64.34
ATOM 1800 O LYS A 935 -12.094 47.221 -22.884 1.00 65.68
ATOM 1801 CB LYS A 935 -9.787 47.316 -20.642 1.00 66.02
ATOM 1802 CG LYS A 935 -9.036 48.128 -19.598 1.00 68.95
ATOM 1803 CD LYS A 935 -8.968 49.594 -19.972 1.00 72.74
ATOM 1804 CE LYS A 935 -7.957 50.327 -19.106 1.00 74.63
ATOM 1805 NZ LYS A 935 -7.835 51.751 -19.525 1.00 76.76
ATOM 1806 N GLY A 936 -12.204 45.422 -21.534 1.00 62.92
ATOM 1807 CA GLY A 936 -12.800 44.578 -22.552 1.00 61.68
ATOM 1808 C GLY A 936 -12.202 43.192 -22.683 1.00 61.72
ATOM 1809 O GLY A 936 -12.830 42.298 -23.250 1.00 61.81
ATOM 1810 N GLU A 937 -10.991 43.013 -22.164 1.00 60.83
ATOM 1811 CA GLU A 937 -10.276 41.734 -22.217 1.00 59.06
ATOM 1812 C GLU A 937 -11.148 40.509 -21.889 1.00 57.16
ATOM 1813 O GLU A 937 -12.066 40.588 -21.073 1.00 56.93
ATOM 1814 CB GLU A 937 -9.086 41.774 -21.245 1.00 59.84
ATOM 1815 CG GLU A 937 -8.222 40.530 -21.268 1.00 62.61
ATOM 1816 CD GLU A 937 -6.844 40.793 -21.823 1.00 64.42
ATOM 1817 OE1 GLU A 937 -6.690 41.760 -22.595 1.00 64.76
ATOM 1818 OE2 GLU A 937 -5.916 40.024 -21.495 1.00 66.97
ATOM 1819 N ARG A 938 -10.842 39.382 -22.528 1.00 54.12
ATOM 1820 CA ARG A 938 -11.561 38.127 -22.311 1.00 51.97
ATOM 1821 C ARG A 938 -10.653 36.961 -22.658 1.00 51.14
ATOM 1822 O ARG A 938 -9.759 37.104 -23.486 1.00 54.50
ATOM 1823 CB ARG A 938 -12.810 38.053 -23.190 1.00 50.05
ATOM 1824 CG ARG A 938 -13.914 38.970 -22.756 1.00 48.91
ATOM 1825 CD ARG A 938 -14.329 38.646 -21.338 1.00 49.76
ATOM 1826 NE ARG A 938 -14.723 39.860 -20.636 1.00 54.12
ATOM 1827 CZ ARG A 938 -15.817 40.555 -20.911 1.00 53.77
ATOM 1828 NH1 ARG A 938 -16.624 40.141 -21.874 1.00 60.00
ATOM 1829 NH2 ARG A 938 -16.104 41.654 -20.235 1.00 48.85
ATOM 1830 N LEU A 939 -10.876 35.810 -22.035 1.00 47.64
ATOM 1831 CA LEU A 939 -10.059 34.647 -22.338 1.00 47.01
ATOM 1832 C LEU A 939 -10.058 34.409 -23.854 1.00 46.67

ATOM 1833 O LEU A 939 -11.041 34.691 -24.539 1.00 45.61
ATOM 1834 CB LEU A 939 -10.591 33.422 -21.587 1.00 46.49
ATOM 1835 CG LEU A 939 -10.427 33.537 -20.065 1.00 45.25
ATOM 1836 CD1 LEU A 939 -11.279 32.505 -19.343 1.00 43.35
ATOM 1837 CD2 LEU A 939 -8.968 33.376 -19.716 1.00 42.97
ATOM 1838 N PRO A 940 -8.943 33.896 -24.397 1.00 46.22
ATOM 1839 CA PRO A 940 -8.749 33.604 -25.826 1.00 44.26
ATOM 1840 C PRO A 940 -9.532 32.402 -26.327 1.00 45.20
ATOM 1841 O PRO A 940 -9.911 31.533 -25.555 1.00 46.46
ATOM 1842 CB PRO A 940 -7.252 33.336 -25.936 1.00 42.34
ATOM 1843 CG PRO A 940 -6.672 33.871 -24.654 1.00 46.14
ATOM 1844 CD PRO A 940 -7.726 33.590 -23.637 1.00 43.98
ATOM 1845 N GLN A 941 -9.737 32.346 -27.637 1.00 46.70
ATOM 1846 CA GLN A 941 -10.448 31.242 -28.263 1.00 46.31
ATOM 1847 C GLN A 941 -9.558 30.012 -28.242 1.00 46.69
ATOM 1848 O GLN A 941 -8.479 30.009 -28.824 1.00 46.60
ATOM 1849 CB GLN A 941 -10.810 31.605 -29.704 1.00 45.70
ATOM 1850 CG GLN A 941 -11.506 30.500 -30.467 1.00 46.44
ATOM 1851 CD GLN A 941 -12.083 30.960 -31.808 1.00 48.60
ATOM 1852 OE1 GLN A 941 -12.721 30.178 -32.521 1.00 47.90
ATOM 1853 NE2 GLN A 941 -11.861 32.226 -32.154 1.00 50.29
ATOM 1854 N PRO A 942 -9.992 28.950 -27.553 1.00 48.40
ATOM 1855 CA PRO A 942 -9.184 27.728 -27.490 1.00 49.09
ATOM 1856 C PRO A 942 -8.955 27.174 -28.894 1.00 50.75
ATOM 1857 O PRO A 942 -9.822 27.268 -29.755 1.00 52.32
ATOM 1858 CB PRO A 942 -10.036 26.793 -26.635 1.00 47.59
ATOM 1859 CG PRO A 942 -10.810 27.745 -25.767 1.00 49.17
ATOM 1860 CD PRO A 942 -11.210 28.822 -26.739 1.00 46.31
ATOM 1861 N PRO A 943 -7.781 26.584 -29.141 1.00 52.29
ATOM 1862 CA PRO A 943 -7.452 26.017 -30.450 1.00 51.87
ATOM 1863 C PRO A 943 -8.535 25.089 -31.025 1.00 52.45
ATOM 1864 O PRO A 943 -9.006 25.300 -32.147 1.00 53.80
ATOM 1865 CB PRO A 943 -6.149 25.270 -30.175 1.00 53.02
ATOM 1866 CG PRO A 943 -5.511 26.097 -29.120 1.00 52.76
ATOM 1867 CD PRO A 943 -6.670 26.391 -28.195 1.00 53.36
ATOM 1868 N ILE A 944 -8.927 24.073 -30.256 1.00 50.16
ATOM 1869 CA ILE A 944 -9.928 23.100 -30.702 1.00 48.57
ATOM 1870 C ILE A 944 -11.349 23.635 -30.776 1.00 49.82
ATOM 1871 O ILE A 944 -12.259 22.953 -31.268 1.00 47.90
ATOM 1872 CB ILE A 944 -9.973 21.876 -29.778 1.00 47.78
ATOM 1873 CG1 ILE A 944 -10.608 22.255 -28.430 1.00 43.48
ATOM 1874 CG2 ILE A 944 -8.579 21.321 -29.607 1.00 46.76
ATOM 1875 CD1 ILE A 944 -10.784 21.080 -27.499 1.00 42.87
ATOM 1876 N CYS A 945 -11.542 24.847 -30.275 1.00 51.05
ATOM 1877 CA CYS A 945 -12.860 25.449 -30.270 1.00 51.69

ATOM 1878 C CYS A 945 -13.254 26.015 -31.604 1.00 52.55
ATOM 1879 O CYS A 945 -12.490 26.739 -32.240 1.00 55.03
ATOM 1880 CB CYS A 945 -12.951 26.557 -29.217 1.00 52.52
ATOM 1881 SG CYS A 945 -13.270 25.971 -27.546 1.00 52.50
ATOM 1882 N THR A 946 -14.465 25.666 -32.011 1.00 51.88
ATOM 1883 CA THR A 946 -15.059 26.138 -33.246 1.00 50.67
ATOM 1884 C THR A 946 -15.703 27.448 -32.793 1.00 49.33
ATOM 1885 O THR A 946 -16.054 27.571 -31.626 1.00 49.43
ATOM 1886 CB THR A 946 -16.126 25.127 -33.733 1.00 50.13
ATOM 1887 OG1 THR A 946 -16.468 25.404 -35.091 1.00 52.85
ATOM 1888 CG2 THR A 946 -17.376 25.205 -32.871 1.00 46.57
ATOM 1889 N ILE A 947 -15.849 28.424 -33.684 1.00 49.50
ATOM 1890 CA ILE A 947 -16.436 29.705 -33.289 1.00 48.83
ATOM 1891 C ILE A 947 -17.843 29.569 -32.718 1.00 49.26
ATOM 1892 O ILE A 947 -18.415 30.527 -32.195 1.00 52.14
ATOM 1893 CB ILE A 947 -16.481 30.714 -34.454 1.00 48.12
ATOM 1894 CG1 ILE A 947 -16.732 32.121 -33.888 1.00 49.16
ATOM 1895 CG2 ILE A 947 -17.570 30.321 -35.452 1.00 46.40
ATOM 1896 CD1 ILE A 947 -16.721 33.247 -34.909 1.00 50.09
ATOM 1897 N ASP A 948 -18.407 28.379 -32.819 1.00 48.28
ATOM 1898 CA ASP A 948 -19.734 28.137 -32.279 1.00 47.63
ATOM 1899 C ASP A 948 -19.621 27.996 -30.761 1.00 46.50
ATOM 1900 O ASP A 948 -20.413 28.583 -30.012 1.00 46.41
ATOM 1901 CB ASP A 948 -20.311 26.857 -32.888 1.00 49.31
ATOM 1902 CG ASP A 948 -20.568 26.988 -34.377 1.00 49.35
ATOM 1903 OD1 ASP A 948 -21.612 27.553 -34.737 1.00 52.88
ATOM 1904 OD2 ASP A 948 -19.729 26.543 -35.186 1.00 50.17
ATOM 1905 N VAL A 949 -18.626 27.226 -30.317 1.00 43.56
ATOM 1906 CA VAL A 949 -18.405 26.998 -28.896 1.00 43.65
ATOM 1907 C VAL A 949 -17.894 28.262 -28.222 1.00 43.64
ATOM 1908 O VAL A 949 -18.333 28.619 -27.127 1.00 44.08
ATOM 1909 CB VAL A 949 -17.381 25.858 -28.654 1.00 43.97
ATOM 1910 CG1 VAL A 949 -17.132 25.689 -27.158 1.00 41.83
ATOM 1911 CG2 VAL A 949 -17.895 24.551 -29.246 1.00 41.36
ATOM 1912 N TYR A 950 -16.965 28.939 -28.885 1.00 43.36
ATOM 1913 CA TYR A 950 -16.395 30.160 -28.343 1.00 42.30
ATOM 1914 C TYR A 950 -17.478 31.180 -28.036 1.00 41.41
ATOM 1915 O TYR A 950 -17.489 31.774 -26.961 1.00 40.32
ATOM 1916 CB TYR A 950 -15.386 30.760 -29.322 1.00 43.03
ATOM 1917 CG TYR A 950 -14.489 31.806 -28.686 1.00 45.66
ATOM 1918 CD1 TYR A 950 -13.837 31.549 -27.473 1.00 45.82
ATOM 1919 CD2 TYR A 950 -14.283 33.044 -29.290 1.00 46.41
ATOM 1920 CE1 TYR A 950 -13.004 32.496 -26.879 1.00 44.71
ATOM 1921 CE2 TYR A 950 -13.446 34.002 -28.701 1.00 47.81
ATOM 1922 CZ TYR A 950 -12.811 33.715 -27.498 1.00 46.62

ATOM 1923 OH TYR A 950 -11.967 34.638 -26.931 1.00 46.10
ATOM 1924 N MET A 951 -18.390 31.386 -28.978 1.00 41.91
ATOM 1925 CA MET A 951 -19.459 32.343 -28.761 1.00 43.90
ATOM 1926 C MET A 951 -20.267 31.988 -27.532 1.00 44.53
ATOM 1927 O MET A 951 -20.776 32.877 -26.849 1.00 47.60
ATOM 1928 CB MET A 951 -20.366 32.447 -29.989 1.00 47.27
ATOM 1929 CG MET A 951 -19.674 33.105 -31.166 1.00 53.88
ATOM 1930 SD MET A 951 -18.776 34.589 -30.618 1.00 62.31
ATOM 1931 CE MET A 951 -20.155 35.487 -29.841 1.00 55.74
ATOM 1932 N VAL A 952 -20.397 30.700 -27.232 1.00 42.77
ATOM 1933 CA VAL A 952 -21.131 30.334 -26.031 1.00 42.94
ATOM 1934 C VAL A 952 -20.352 30.869 -24.819 1.00 44.09
ATOM 1935 O VAL A 952 -20.928 31.493 -23.923 1.00 44.56
ATOM 1936 CB VAL A 952 -21.341 28.795 -25.924 1.00 42.99
ATOM 1937 CG1 VAL A 952 -21.891 28.430 -24.551 1.00 39.35
ATOM 1938 CG2 VAL A 952 -22.332 28.339 -26.999 1.00 39.89
ATOM 1939 N MET A 953 -19.039 30.654 -24.807 1.00 44.23
ATOM 1940 CA MET A 953 -18.202 31.142 -23.711 1.00 45.49
ATOM 1941 C MET A 953 -18.231 32.670 -23.603 1.00 45.43
ATOM 1942 O MET A 953 -18.393 33.225 -22.510 1.00 45.00
ATOM 1943 CB MET A 953 -16.759 30.683 -23.900 1.00 44.82
ATOM 1944 CG MET A 953 -16.587 29.199 -23.816 1.00 48.13
ATOM 1945 SD MET A 953 -14.944 28.724 -24.267 1.00 52.76
ATOM 1946 CE MET A 953 -15.146 26.965 -24.437 1.00 52.38
ATOM 1947 N VAL A 954 -18.081 33.353 -24.734 1.00 42.69
ATOM 1948 CA VAL A 954 -18.086 34.804 -24.705 1.00 42.88
ATOM 1949 C VAL A 954 -19.408 35.363 -24.175 1.00 43.39
ATOM 1950 O VAL A 954 -19.402 36.290 -23.381 1.00 44.32
ATOM 1951 CB VAL A 954 -17.792 35.394 -26.090 1.00 42.98
ATOM 1952 CG1 VAL A 954 -17.863 36.890 -26.020 1.00 44.13
ATOM 1953 CG2 VAL A 954 -16.403 34.961 -26.565 1.00 43.05
ATOM 1954 N LYS A 955 -20.545 34.812 -24.589 1.00 43.09
ATOM 1955 CA LYS A 955 -21.814 35.327 -24.070 1.00 44.12
ATOM 1956 C LYS A 955 -21.844 35.189 -22.552 1.00 43.87
ATOM 1957 O LYS A 955 -22.417 36.024 -21.855 1.00 44.04
ATOM 1958 CB LYS A 955 -23.012 34.573 -24.656 1.00 45.68
ATOM 1959 CG LYS A 955 -23.304 34.831 -26.123 1.00 46.27
ATOM 1960 CD LYS A 955 -24.430 33.924 -26.563 1.00 46.94
ATOM 1961 CE LYS A 955 -24.660 33.965 -28.048 1.00 50.31
ATOM 1962 NZ LYS A 955 -25.433 32.759 -28.442 1.00 51.04
ATOM 1963 N CYS A 956 -21.238 34.123 -22.042 1.00 43.06
ATOM 1964 CA CYS A 956 -21.199 33.896 -20.602 1.00 43.04
ATOM 1965 C CYS A 956 -20.505 35.042 -19.861 1.00 44.88
ATOM 1966 O CYS A 956 -20.712 35.235 -18.652 1.00 42.74
ATOM 1967 CB CYS A 956 -20.453 32.606 -20.296 1.00 40.76

ATOM 1968 SG CYS A 956 -21.406 31.114 -20.517 1.00 40.75
ATOM 1969 N TRP A 957 -19.684 35.796 -20.593 1.00 46.16
ATOM 1970 CA TRP A 957 -18.929 36.888 -20.006 1.00 47.28
ATOM 1971 C TRP A 957 -19.409 38.283 -20.373 1.00 49.59
ATOM 1972 O TRP A 957 -18.629 39.231 -20.342 1.00 50.87
ATOM 1973 CB TRP A 957 -17.442 36.749 -20.365 1.00 44.94
ATOM 1974 CG TRP A 957 -16.881 35.389 -20.062 1.00 41.87
ATOM 1975 CD1 TRP A 957 -17.113 34.636 -18.949 1.00 40.97
ATOM 1976 CD2 TRP A 957 -15.987 34.628 -20.880 1.00 40.66
ATOM 1977 NE1 TRP A 957 -16.423 33.450 -19.022 1.00 41.10
ATOM 1978 CE2 TRP A 957 -15.720 33.419 -20.196 1.00 39.58
ATOM 1979 CE3 TRP A 957 -15.383 34.850 -22.125 1.00 39.57
ATOM 1980 CZ2 TRP A 957 -14.877 32.435 -20.712 1.00 39.64
ATOM 1981 CZ3 TRP A 957 -14.545 33.871 -22.639 1.00 40.43
ATOM 1982 CH2 TRP A 957 -14.298 32.676 -21.930 1.00 40.43
ATOM 1983 N MET A 958 -20.682 38.425 -20.720 1.00 50.92
ATOM 1984 CA MET A 958 -21.186 39.752 -21.048 1.00 52.62
ATOM 1985 C MET A 958 -21.165 40.609 -19.789 1.00 50.99
ATOM 1986 O MET A 958 -21.272 40.098 -18.676 1.00 49.32
ATOM 1987 CB MET A 958 -22.609 39.682 -21.598 1.00 54.02
ATOM 1988 CG MET A 958 -22.708 38.991 -22.941 1.00 57.72
ATOM 1989 SD MET A 958 -21.589 39.707 -24.136 1.00 61.72
ATOM 1990 CE MET A 958 -22.626 41.096 -24.754 1.00 62.55
ATOM 1991 N ILE A 959 -21.009 41.913 -19.968 1.00 51.63
ATOM 1992 CA ILE A 959 -20.979 42.819 -18.829 1.00 53.09
ATOM 1993 C ILE A 959 -22.342 42.742 -18.161 1.00 52.72
ATOM 1994 O ILE A 959 -22.461 42.808 -16.944 1.00 52.77
ATOM 1995 CB ILE A 959 -20.740 44.273 -19.267 1.00 53.98
ATOM 1996 CG1 ILE A 959 -19.387 44.387 -19.981 1.00 57.72
ATOM 1997 CG2 ILE A 959 -20.785 45.191 -18.050 1.00 53.54
ATOM 1998 CD1 ILE A 959 -19.163 45.733 -20.703 1.00 60.53
ATOM 1999 N ASP A 960 -23.374 42.584 -18.977 1.00 53.04
ATOM 2000 CA ASP A 960 -24.733 42.505 -18.472 1.00 54.30
ATOM 2001 C ASP A 960 -25.075 41.102 -17.961 1.00 53.33
ATOM 2002 O ASP A 960 -25.337 40.191 -18.739 1.00 50.47
ATOM 2003 CB ASP A 960 -25.706 42.903 -19.575 1.00 57.50
ATOM 2004 CG ASP A 960 -26.971 43.511 -19.035 1.00 59.92
ATOM 2005 OD1 ASP A 960 -27.626 42.880 -18.177 1.00 63.64
ATOM 2006 OD2 ASP A 960 -27.312 44.626 -19.476 1.00 62.47
ATOM 2007 N ALA A 961 -25.077 40.942 -16.646 1.00 53.51
ATOM 2008 CA ALA A 961 -25.384 39.659 -16.033 1.00 54.51
ATOM 2009 C ALA A 961 -26.650 39.046 -16.637 1.00 55.26
ATOM 2010 O ALA A 961 -26.690 37.856 -16.956 1.00 53.76
ATOM 2011 CB ALA A 961 -25.549 39.839 -14.528 1.00 52.04
ATOM 2012 N ASP A 962 -27.677 39.870 -16.804 1.00 56.69

```
ATOM  2013  CA  ASP A 962     -28.942  39.405 -17.360  1.00 58.69
ATOM  2014  C   ASP A 962     -28.948  38.994 -18.830  1.00 57.34
ATOM  2015  O   ASP A 962     -29.803  38.211 -19.241  1.00 57.60
ATOM  2016  CB  ASP A 962     -30.043  40.439 -17.118  1.00 61.14
ATOM  2017  CG  ASP A 962     -30.633  40.339 -15.724  1.00 64.05
ATOM  2018  OD1 ASP A 962     -30.863  39.199 -15.259  1.00 62.71
ATOM  2019  OD2 ASP A 962     -30.876  41.396 -15.103  1.00 68.35
ATOM  2020  N   SER A 963     -28.022  39.509 -19.631  1.00 56.01
ATOM  2021  CA  SER A 963     -27.996  39.111 -21.031  1.00 54.55
ATOM  2022  C   SER A 963     -27.117  37.870 -21.249  1.00 53.95
ATOM  2023  O   SER A 963     -26.940  37.415 -22.378  1.00 55.77
ATOM  2024  CB  SER A 963     -27.537  40.275 -21.925  1.00 55.92
ATOM  2025  OG  SER A 963     -26.176  40.600 -21.734  1.00 55.38
ATOM  2026  N   ARG A 964     -26.565  37.323 -20.170  1.00 51.26
ATOM  2027  CA  ARG A 964     -25.746  36.115 -20.272  1.00 50.44
ATOM  2028  C   ARG A 964     -26.711  34.942 -20.410  1.00 50.43
ATOM  2029  O   ARG A 964     -27.820  34.970 -19.874  1.00 50.63
ATOM  2030  CB  ARG A 964     -24.899  35.900 -19.010  1.00 47.22
ATOM  2031  CG  ARG A 964     -23.902  36.994 -18.724  1.00 45.09
ATOM  2032  CD  ARG A 964     -23.324  36.875 -17.329  1.00 42.47
ATOM  2033  NE  ARG A 964     -22.590  38.085 -16.981  1.00 44.27
ATOM  2034  CZ  ARG A 964     -22.156  38.392 -15.761  1.00 43.66
ATOM  2035  NH1 ARG A 964     -22.368  37.577 -14.736  1.00 38.19
ATOM  2036  NH2 ARG A 964     -21.527  39.543 -15.567  1.00 43.56
ATOM  2037  N   PRO A 965     -26.303  33.891 -21.126  1.00 50.03
ATOM  2038  CA  PRO A 965     -27.230  32.762 -21.256  1.00 50.55
ATOM  2039  C   PRO A 965     -27.593  32.164 -19.890  1.00 50.02
ATOM  2040  O   PRO A 965     -26.851  32.318 -18.920  1.00 50.28
ATOM  2041  CB  PRO A 965     -26.460  31.786 -22.146  1.00 49.94
ATOM  2042  CG  PRO A 965     -25.011  32.123 -21.855  1.00 51.67
ATOM  2043  CD  PRO A 965     -25.011  33.617 -21.780  1.00 49.61
ATOM  2044  N   LYS A 966     -28.748  31.515 -19.804  1.00 48.80
ATOM  2045  CA  LYS A 966     -29.153  30.889 -18.554  1.00 48.28
ATOM  2046  C   LYS A 966     -28.753  29.418 -18.572  1.00 47.56
ATOM  2047  O   LYS A 966     -28.629  28.808 -19.642  1.00 45.03
ATOM  2048  CB  LYS A 966     -30.654  31.021 -18.343  1.00 49.99
ATOM  2049  CG  LYS A 966     -31.096  32.436 -18.067  1.00 55.88
ATOM  2050  CD  LYS A 966     -32.242  32.462 -17.073  1.00 60.89
ATOM  2051  CE  LYS A 966     -32.579  33.893 -16.660  1.00 64.65
ATOM  2052  NZ  LYS A 966     -33.599  33.951 -15.563  1.00 65.07
ATOM  2053  N   PHE A 967     -28.546  28.842 -17.392  1.00 45.93
ATOM  2054  CA  PHE A 967     -28.138  27.449 -17.327  1.00 46.66
ATOM  2055  C   PHE A 967     -29.005  26.499 -18.135  1.00 47.20
ATOM  2056  O   PHE A 967     -28.518  25.470 -18.579  1.00 49.36
ATOM  2057  CB  PHE A 967     -28.029  26.988 -15.875  1.00 46.03
```

ATOM 2058 CG PHE A 967 -26.767 27.437 -15.213 1.00 45.56
ATOM 2059 CD1 PHE A 967 -26.792 28.392 -14.199 1.00 45.88
ATOM 2060 CD2 PHE A 967 -25.535 26.971 -15.669 1.00 44.49
ATOM 2061 CE1 PHE A 967 -25.599 28.886 -13.650 1.00 47.81
ATOM 2062 CE2 PHE A 967 -24.340 27.455 -15.131 1.00 46.71
ATOM 2063 CZ PHE A 967 -24.368 28.416 -14.119 1.00 45.70
ATOM 2064 N ALA A 968 -30.275 26.846 -18.340 1.00 47.85
ATOM 2065 CA ALA A 968 -31.183 26.014 -19.136 1.00 48.27
ATOM 2066 C ALA A 968 -30.746 25.988 -20.615 1.00 49.39
ATOM 2067 O ALA A 968 -30.753 24.943 -21.264 1.00 49.53
ATOM 2068 CB ALA A 968 -32.620 26.542 -19.028 1.00 45.49
ATOM 2069 N GLU A 969 -30.358 27.142 -21.144 1.00 49.32
ATOM 2070 CA GLU A 969 -29.939 27.226 -22.533 1.00 48.74
ATOM 2071 C GLU A 969 -28.574 26.587 -22.760 1.00 48.05
ATOM 2072 O GLU A 969 -28.325 25.986 -23.812 1.00 47.73
ATOM 2073 CB GLU A 969 -29.863 28.682 -22.976 1.00 51.47
ATOM 2074 CG GLU A 969 -31.120 29.492 -22.779 1.00 55.25
ATOM 2075 CD GLU A 969 -30.928 30.929 -23.246 1.00 60.64
ATOM 2076 OE1 GLU A 969 -30.233 31.703 -22.539 1.00 58.91
ATOM 2077 OE2 GLU A 969 -31.454 31.274 -24.335 1.00 63.69
ATOM 2078 N LEU A 970 -27.681 26.739 -21.784 1.00 44.93
ATOM 2079 CA LEU A 970 -26.343 26.186 -21.918 1.00 42.24
ATOM 2080 C LEU A 970 -26.430 24.686 -22.019 1.00 41.43
ATOM 2081 O LEU A 970 -25.822 24.081 -22.901 1.00 40.90
ATOM 2082 CB LEU A 970 -25.450 26.611 -20.741 1.00 40.56
ATOM 2083 CG LEU A 970 -25.011 28.089 -20.768 1.00 37.75
ATOM 2084 CD1 LEU A 970 -24.376 28.470 -19.459 1.00 37.42
ATOM 2085 CD2 LEU A 970 -24.058 28.329 -21.906 1.00 32.61
ATOM 2086 N ALA A 971 -27.207 24.079 -21.134 1.00 41.36
ATOM 2087 CA ALA A 971 -27.350 22.634 -21.175 1.00 42.61
ATOM 2088 C ALA A 971 -27.934 22.243 -22.518 1.00 44.03
ATOM 2089 O ALA A 971 -27.470 21.309 -23.162 1.00 44.82
ATOM 2090 CB ALA A 971 -28.252 22.168 -20.074 1.00 42.94
ATOM 2091 N ALA A 972 -28.948 22.980 -22.941 1.00 43.93
ATOM 2092 CA ALA A 972 -29.600 22.705 -24.200 1.00 46.31
ATOM 2093 C ALA A 972 -28.675 22.874 -25.411 1.00 49.37
ATOM 2094 O ALA A 972 -28.638 22.013 -26.300 1.00 51.33
ATOM 2095 CB ALA A 972 -30.825 23.601 -24.342 1.00 43.28
ATOM 2096 N GLU A 973 -27.934 23.976 -25.454 1.00 50.72
ATOM 2097 CA GLU A 973 -27.045 24.243 -26.580 1.00 52.77
ATOM 2098 C GLU A 973 -25.930 23.205 -26.699 1.00 51.88
ATOM 2099 O GLU A 973 -25.721 22.643 -27.768 1.00 52.95
ATOM 2100 CB GLU A 973 -26.463 25.662 -26.450 1.00 57.46
ATOM 2101 CG GLU A 973 -25.475 26.119 -27.540 1.00 62.52
ATOM 2102 CD GLU A 973 -26.081 26.196 -28.944 1.00 67.05

ATOM 2103 OE1 GLU A 973 -27.304 26.435 -29.067 1.00 69.19
ATOM 2104 OE2 GLU A 973 -25.323 26.032 -29.930 1.00 68.06
ATOM 2105 N PHE A 974 -25.219 22.935 -25.609 1.00 49.75
ATOM 2106 CA PHE A 974 -24.134 21.965 -25.679 1.00 48.22
ATOM 2107 C PHE A 974 -24.698 20.605 -25.979 1.00 47.87
ATOM 2108 O PHE A 974 -24.088 19.806 -26.678 1.00 47.01
ATOM 2109 CB PHE A 974 -23.345 21.938 -24.374 1.00 46.42
ATOM 2110 CG PHE A 974 -22.362 23.053 -24.258 1.00 47.75
ATOM 2111 CD1 PHE A 974 -21.276 23.129 -25.128 1.00 48.10
ATOM 2112 CD2 PHE A 974 -22.547 24.071 -23.327 1.00 47.47
ATOM 2113 CE1 PHE A 974 -20.390 24.204 -25.077 1.00 46.79
ATOM 2114 CE2 PHE A 974 -21.673 25.148 -23.270 1.00 47.11
ATOM 2115 CZ PHE A 974 -20.588 25.215 -24.150 1.00 47.33
ATOM 2116 N SER A 975 -25.886 20.360 -25.446 1.00 47.80
ATOM 2117 CA SER A 975 -26.581 19.102 -25.644 1.00 47.24
ATOM 2118 C SER A 975 -26.704 18.813 -27.136 1.00 47.38
ATOM 2119 O SER A 975 -26.389 17.708 -27.588 1.00 47.22
ATOM 2120 CB SER A 975 -27.976 19.182 -25.022 1.00 48.16
ATOM 2121 OG SER A 975 -28.591 17.914 -24.947 1.00 49.36
ATOM 2122 N ARG A 976 -27.158 19.796 -27.910 1.00 45.99
ATOM 2123 CA ARG A 976 -27.301 19.558 -29.335 1.00 46.51
ATOM 2124 C ARG A 976 -25.925 19.475 -30.004 1.00 46.75
ATOM 2125 O ARG A 976 -25.779 18.840 -31.042 1.00 47.59
ATOM 2126 CB ARG A 976 -28.189 20.633 -29.988 1.00 44.73
ATOM 2127 CG ARG A 976 -27.436 21.795 -30.545 1.00 50.21
ATOM 2128 CD ARG A 976 -28.301 22.825 -31.270 1.00 51.39
ATOM 2129 NE ARG A 976 -27.435 23.946 -31.634 1.00 53.87
ATOM 2130 CZ ARG A 976 -26.509 23.885 -32.587 1.00 54.84
ATOM 2131 NH1 ARG A 976 -25.740 24.936 -32.849 1.00 56.13
ATOM 2132 NH2 ARG A 976 -26.383 22.784 -33.313 1.00 52.91
ATOM 2133 N MET A 977 -24.909 20.090 -29.406 1.00 48.59
ATOM 2134 CA MET A 977 -23.562 20.036 -29.979 1.00 50.45
ATOM 2135 C MET A 977 -22.996 18.635 -29.790 1.00 51.16
ATOM 2136 O MET A 977 -22.230 18.140 -30.620 1.00 51.33
ATOM 2137 CB MET A 977 -22.637 21.080 -29.324 1.00 51.44
ATOM 2138 CG MET A 977 -22.833 22.507 -29.861 1.00 54.98
ATOM 2139 SD MET A 977 -22.111 23.823 -28.853 1.00 58.42
ATOM 2140 CE MET A 977 -20.982 24.513 -29.911 1.00 56.62
ATOM 2141 N ALA A 978 -23.399 17.990 -28.703 1.00 51.59
ATOM 2142 CA ALA A 978 -22.938 16.646 -28.395 1.00 52.55
ATOM 2143 C ALA A 978 -23.492 15.596 -29.363 1.00 53.68
ATOM 2144 O ALA A 978 -22.947 14.501 -29.477 1.00 54.76
ATOM 2145 CB ALA A 978 -23.312 16.292 -26.959 1.00 50.13
ATOM 2146 N ARG A 979 -24.573 15.922 -30.058 1.00 55.30
ATOM 2147 CA ARG A 979 -25.156 14.983 -31.006 1.00 58.64

```
ATOM   2148  C   ARG A 979     -24.312  14.943 -32.279  1.00 59.72
ATOM   2149  O   ARG A 979     -24.554  14.127 -33.166  1.00 60.30
ATOM   2150  CB  ARG A 979     -26.586  15.397 -31.370  1.00 60.38
ATOM   2151  CG  ARG A 979     -27.545  15.474 -30.195  1.00 65.31
ATOM   2152  CD  ARG A 979     -28.864  16.123 -30.604  1.00 67.03
ATOM   2153  NE  ARG A 979     -29.575  16.664 -29.448  1.00 68.78
ATOM   2154  CZ  ARG A 979     -30.539  17.581 -29.516  1.00 70.15
ATOM   2155  NH1 ARG A 979     -30.922  18.067 -30.694  1.00 70.75
ATOM   2156  NH2 ARG A 979     -31.107  18.027 -28.398  1.00 70.11
ATOM   2157  N   ASP A 980     -23.325  15.827 -32.365  1.00 59.38
ATOM   2158  CA  ASP A 980     -22.464  15.903 -33.541  1.00 59.02
ATOM   2159  C   ASP A 980     -21.190  16.645 -33.122  1.00 57.66
ATOM   2160  O   ASP A 980     -20.858  17.709 -33.649  1.00 56.21
ATOM   2161  CB  ASP A 980     -23.215  16.654 -34.649  1.00 60.77
ATOM   2162  CG  ASP A 980     -22.502  16.607 -35.990  1.00 62.49
ATOM   2163  OD1 ASP A 980     -21.643  15.717 -36.183  1.00 64.46
ATOM   2164  OD2 ASP A 980     -22.821  17.456 -36.858  1.00 61.55
ATOM   2165  N   PRO A 981     -20.453  16.066 -32.162  1.00 56.22
ATOM   2166  CA  PRO A 981     -19.208  16.598 -31.598  1.00 55.44
ATOM   2167  C   PRO A 981     -18.084  17.037 -32.535  1.00 53.93
ATOM   2168  O   PRO A 981     -17.492  18.090 -32.323  1.00 53.34
ATOM   2169  CB  PRO A 981     -18.772  15.496 -30.629  1.00 55.07
ATOM   2170  CG  PRO A 981     -19.345  14.262 -31.229  1.00 54.89
ATOM   2171  CD  PRO A 981     -20.718  14.715 -31.637  1.00 55.91
ATOM   2172  N   GLN A 982     -17.773  16.245 -33.556  1.00 54.01
ATOM   2173  CA  GLN A 982     -16.698  16.617 -34.476  1.00 53.13
ATOM   2174  C   GLN A 982     -17.043  17.886 -35.253  1.00 50.44
ATOM   2175  O   GLN A 982     -16.188  18.476 -35.897  1.00 48.82
ATOM   2176  CB  GLN A 982     -16.377  15.470 -35.445  1.00 55.75
ATOM   2177  CG  GLN A 982     -15.535  14.333 -34.851  1.00 59.04
ATOM   2178  CD  GLN A 982     -16.299  13.465 -33.854  1.00 63.65
ATOM   2179  OE1 GLN A 982     -17.524  13.576 -33.721  1.00 65.05
ATOM   2180  NE2 GLN A 982     -15.578  12.605 -33.140  1.00 65.14
ATOM   2181  N   ARG A 983     -18.296  18.311 -35.179  1.00 49.29
ATOM   2182  CA  ARG A 983     -18.716  19.528 -35.861  1.00 49.03
ATOM   2183  C   ARG A 983     -18.482  20.771 -35.012  1.00 47.62
ATOM   2184  O   ARG A 983     -18.549  21.890 -35.514  1.00 48.25
ATOM   2185  CB  ARG A 983     -20.196  19.479 -36.200  1.00 50.98
ATOM   2186  CG  ARG A 983     -20.683  20.768 -36.834  1.00 53.68
ATOM   2187  CD  ARG A 983     -22.171  20.801 -36.932  1.00 55.23
ATOM   2188  NE  ARG A 983     -22.623  21.823 -37.864  1.00 57.30
ATOM   2189  CZ  ARG A 983     -23.903  22.094 -38.081  1.00 58.03
ATOM   2190  NH1 ARG A 983     -24.838  21.416 -37.424  1.00 59.36
ATOM   2191  NH2 ARG A 983     -24.247  23.028 -38.954  1.00 57.21
ATOM   2192  N   TYR A 984     -18.217  20.585 -33.727  1.00 46.14
```

```
ATOM   2193  CA  TYR A 984     -18.005  21.728 -32.860  1.00 46.62
ATOM   2194  C   TYR A 984     -16.629  21.830 -32.178  1.00 45.34
ATOM   2195  O   TYR A 984     -16.165  22.923 -31.866  1.00 44.15
ATOM   2196  CB  TYR A 984     -19.162  21.797 -31.855  1.00 45.73
ATOM   2197  CG  TYR A 984     -20.483  22.095 -32.545  1.00 47.52
ATOM   2198  CD1 TYR A 984     -21.367  21.075 -32.892  1.00 49.29
ATOM   2199  CD2 TYR A 984     -20.816  23.401 -32.920  1.00 47.84
ATOM   2200  CE1 TYR A 984     -22.553  21.352 -33.598  1.00 48.94
ATOM   2201  CE2 TYR A 984     -21.987  23.683 -33.622  1.00 47.24
ATOM   2202  CZ  TYR A 984     -22.847  22.658 -33.957  1.00 48.48
ATOM   2203  OH  TYR A 984     -23.996  22.944 -34.655  1.00 50.81
ATOM   2204  N   LEU A 985     -15.976  20.698 -31.957  1.00 44.95
ATOM   2205  CA  LEU A 985     -14.648  20.689 -31.353  1.00 45.72
ATOM   2206  C   LEU A 985     -13.746  19.932 -32.320  1.00 47.79
ATOM   2207  O   LEU A 985     -14.094  18.836 -32.770  1.00 47.32
ATOM   2208  CB  LEU A 985     -14.672  19.980 -29.997  1.00 44.68
ATOM   2209  CG  LEU A 985     -15.410  20.665 -28.849  1.00 44.43
ATOM   2210  CD1 LEU A 985     -15.243  19.853 -27.574  1.00 43.38
ATOM   2211  CD2 LEU A 985     -14.860  22.079 -28.660  1.00 44.96
ATOM   2212  N   VAL A 986     -12.596  20.510 -32.647  1.00 48.85
ATOM   2213  CA  VAL A 986     -11.679  19.871 -33.582  1.00 49.84
ATOM   2214  C   VAL A 986     -10.398  19.397 -32.911  1.00 51.24
ATOM   2215  O   VAL A 986      -9.426  20.136 -32.805  1.00 51.87
ATOM   2216  CB  VAL A 986     -11.312  20.828 -34.716  1.00 51.14
ATOM   2217  CG1 VAL A 986     -10.392  20.130 -35.709  1.00 50.04
ATOM   2218  CG2 VAL A 986     -12.573  21.325 -35.394  1.00 49.84
ATOM   2219  N   ILE A 987     -10.406  18.146 -32.473  1.00 53.09
ATOM   2220  CA  ILE A 987      -9.267  17.541 -31.797  1.00 52.98
ATOM   2221  C   ILE A 987      -8.535  16.595 -32.736  1.00 55.59
ATOM   2222  O   ILE A 987      -9.155  15.754 -33.392  1.00 53.71
ATOM   2223  CB  ILE A 987      -9.735  16.727 -30.591  1.00 50.88
ATOM   2224  CG1 ILE A 987     -10.571  17.611 -29.665  1.00 52.22
ATOM   2225  CG2 ILE A 987      -8.549  16.124 -29.884  1.00 49.91
ATOM   2226  CD1 ILE A 987     -11.307  16.840 -28.586  1.00 49.45
ATOM   2227  N   GLN A 988      -7.214  16.723 -32.792  1.00 59.02
ATOM   2228  CA  GLN A 988      -6.418  15.860 -33.645  1.00 61.68
ATOM   2229  C   GLN A 988      -6.654  14.424 -33.178  1.00 64.13
ATOM   2230  O   GLN A 988      -6.577  14.127 -31.980  1.00 62.70
ATOM   2231  CB  GLN A 988      -4.946  16.236 -33.528  1.00 63.64
ATOM   2232  CG  GLN A 988      -4.134  15.850 -34.745  1.00 67.15
ATOM   2233  CD  GLN A 988      -2.726  16.407 -34.726  1.00 67.61
ATOM   2234  OE1 GLN A 988      -1.961  16.193 -35.659  1.00 71.31
ATOM   2235  NE2 GLN A 988      -2.378  17.124 -33.665  1.00 70.34
ATOM   2236  N   GLY A 989      -6.947  13.542 -34.131  1.00 66.36
ATOM   2237  CA  GLY A 989      -7.240  12.156 -33.809  1.00 68.95
```

```
ATOM   2238  C   GLY A 989     -8.751  12.071 -33.788  1.00 71.82
ATOM   2239  O   GLY A 989     -9.386  12.067 -34.840  1.00 73.55
ATOM   2240  N   ASP A 990     -9.317  12.011 -32.586  1.00 74.05
ATOM   2241  CA  ASP A 990    -10.766  11.986 -32.362  1.00 75.83
ATOM   2242  C   ASP A 990    -11.591  11.562 -33.583  1.00 77.60
ATOM   2243  O   ASP A 990    -12.564  12.219 -33.951  1.00 77.72
ATOM   2244  CB  ASP A 990    -11.194  13.387 -31.870  1.00 73.28
ATOM   2245  CG  ASP A 990    -12.647  13.457 -31.412  1.00 70.03
ATOM   2246  OD1 ASP A 990    -13.121  12.530 -30.715  1.00 70.19
ATOM   2247  OD2 ASP A 990    -13.308  14.466 -31.732  1.00 65.64
ATOM   2248  N   ALA A 991    -11.208  10.456 -34.208  1.00 80.41
ATOM   2249  CA  ALA A 991    -11.936   9.974 -35.374  1.00 83.98
ATOM   2250  C   ALA A 991    -12.676   8.672 -35.059  1.00 86.60
ATOM   2251  O   ALA A 991    -13.837   8.503 -35.441  1.00 87.41
ATOM   2252  CB  ALA A 991    -10.972   9.771 -36.550  1.00 82.75
ATOM   2253  N   ALA A 992    -12.005   7.767 -34.347  1.00 88.48
ATOM   2254  CA  ALA A 992    -12.582   6.471 -33.992  1.00 90.40
ATOM   2255  C   ALA A 992    -12.798   6.298 -32.492  1.00 91.49
ATOM   2256  O   ALA A 992    -13.875   5.784 -32.113  1.00 91.08
ATOM   2257  CB  ALA A 992    -11.694   5.350 -34.516  1.00 90.58
ATOM   2258  OXT ALA A 992    -11.879   6.655 -31.721  1.00 92.46
ATOM   2259  N   ALA B 694    -21.367   6.079 -64.456  1.00 78.72
ATOM   2260  CA  ALA B 694    -22.190   6.371 -63.252  1.00 78.66
ATOM   2261  C   ALA B 694    -21.358   7.182 -62.263  1.00 78.89
ATOM   2262  O   ALA B 694    -20.424   7.882 -62.653  1.00 79.39
ATOM   2263  CB  ALA B 694    -22.652   5.062 -62.614  1.00 77.87
ATOM   2264  N   ALA B 695    -21.703   7.085 -60.984  1.00 78.95
ATOM   2265  CA  ALA B 695    -20.990   7.791 -59.923  1.00 78.98
ATOM   2266  C   ALA B 695    -20.828   6.832 -58.742  1.00 79.45
ATOM   2267  O   ALA B 695    -21.816   6.296 -58.240  1.00 80.20
ATOM   2268  CB  ALA B 695    -21.775   9.030 -59.498  1.00 77.61
ATOM   2269  N   ALA B 696    -19.588   6.618 -58.305  1.00 79.38
ATOM   2270  CA  ALA B 696    -19.298   5.702 -57.200  1.00 79.53
ATOM   2271  C   ALA B 696    -20.251   5.840 -56.006  1.00 80.35
ATOM   2272  O   ALA B 696    -20.595   6.950 -55.604  1.00 80.03
ATOM   2273  CB  ALA B 696    -17.849   5.883 -56.742  1.00 77.04
ATOM   2274  N   PRO B 697    -20.699   4.701 -55.435  1.00 81.52
ATOM   2275  CA  PRO B 697    -21.611   4.620 -54.284  1.00 81.54
ATOM   2276  C   PRO B 697    -21.046   5.326 -53.053  1.00 82.10
ATOM   2277  O   PRO B 697    -19.916   5.067 -52.635  1.00 82.80
ATOM   2278  CB  PRO B 697    -21.752   3.118 -54.058  1.00 81.54
ATOM   2279  CG  PRO B 697    -21.616   2.564 -55.434  1.00 82.60
ATOM   2280  CD  PRO B 697    -20.452   3.355 -55.987  1.00 82.37
ATOM   2281  N   LEU B 698    -21.845   6.207 -52.467  1.00 81.85
ATOM   2282  CA  LEU B 698    -21.421   6.969 -51.303  1.00 80.76
```

ATOM 2283 C LEU B 698 -21.365 6.109 -50.051 1.00 79.77
ATOM 2284 O LEU B 698 -21.874 4.994 -50.048 1.00 80.40
ATOM 2285 CB LEU B 698 -22.383 8.136 -51.093 1.00 80.50
ATOM 2286 CG LEU B 698 -22.038 9.096 -49.959 1.00 80.61
ATOM 2287 CD1 LEU B 698 -20.711 9.781 -50.243 1.00 80.34
ATOM 2288 CD2 LEU B 698 -23.150 10.118 -49.823 1.00 80.62
ATOM 2289 N THR B 699 -20.732 6.641 -49.006 1.00 79.28
ATOM 2290 CA THR B 699 -20.585 5.992 -47.692 1.00 79.67
ATOM 2291 C THR B 699 -19.385 6.573 -46.938 1.00 78.91
ATOM 2292 O THR B 699 -18.317 5.969 -46.894 1.00 79.37
ATOM 2293 CB THR B 699 -20.408 4.444 -47.792 1.00 80.11
ATOM 2294 OG1 THR B 699 -19.202 4.135 -48.503 1.00 80.37
ATOM 2295 CG2 THR B 699 -21.616 3.801 -48.481 1.00 78.91
ATOM 2296 N PRO B 700 -19.555 7.757 -46.324 1.00 78.42
ATOM 2297 CA PRO B 700 -18.508 8.454 -45.566 1.00 78.09
ATOM 2298 C PRO B 700 -17.960 7.713 -44.354 1.00 77.41
ATOM 2299 O PRO B 700 -18.560 6.759 -43.863 1.00 77.46
ATOM 2300 CB PRO B 700 -19.182 9.764 -45.176 1.00 77.99
ATOM 2301 CG PRO B 700 -20.601 9.355 -45.002 1.00 78.57
ATOM 2302 CD PRO B 700 -20.833 8.482 -46.218 1.00 78.31
ATOM 2303 N SER B 701 -16.811 8.175 -43.876 1.00 76.96
ATOM 2304 CA SER B 701 -16.150 7.577 -42.725 1.00 76.79
ATOM 2305 C SER B 701 -15.878 8.645 -41.676 1.00 76.45
ATOM 2306 O SER B 701 -16.079 9.838 -41.920 1.00 76.52
ATOM 2307 CB SER B 701 -14.824 6.944 -43.154 1.00 77.52
ATOM 2308 OG SER B 701 -13.944 7.924 -43.690 1.00 77.51
ATOM 2309 N GLY B 702 -15.418 8.221 -40.507 1.00 75.81
ATOM 2310 CA GLY B 702 -15.123 9.188 -39.466 1.00 75.42
ATOM 2311 C GLY B 702 -14.011 10.118 -39.912 1.00 73.55
ATOM 2312 O GLY B 702 -14.195 11.334 -40.015 1.00 73.83
ATOM 2313 N THR B 703 -12.858 9.521 -40.194 1.00 71.08
ATOM 2314 CA THR B 703 -11.662 10.227 -40.629 1.00 68.76
ATOM 2315 C THR B 703 -11.903 11.547 -41.346 1.00 66.14
ATOM 2316 O THR B 703 -12.657 11.616 -42.309 1.00 66.70
ATOM 2317 CB THR B 703 -10.826 9.341 -41.553 1.00 70.67
ATOM 2318 OG1 THR B 703 -10.649 8.051 -40.948 1.00 72.31
ATOM 2319 CG2 THR B 703 -9.466 9.982 -41.809 1.00 71.40
ATOM 2320 N ALA B 704 -11.244 12.596 -40.871 1.00 62.68
ATOM 2321 CA ALA B 704 -11.370 13.915 -41.469 1.00 59.07
ATOM 2322 C ALA B 704 -10.277 14.034 -42.529 1.00 57.68
ATOM 2323 O ALA B 704 -9.333 13.236 -42.556 1.00 56.92
ATOM 2324 CB ALA B 704 -11.210 14.992 -40.403 1.00 56.44
ATOM 2325 N PRO B 705 -10.387 15.030 -43.418 1.00 54.82
ATOM 2326 CA PRO B 705 -9.393 15.215 -44.473 1.00 53.14
ATOM 2327 C PRO B 705 -8.001 15.562 -43.982 1.00 52.08

ATOM 2328 O PRO B 705 -7.835 16.297 -43.019 1.00 52.38
ATOM 2329 CB PRO B 705 -9.995 16.328 -45.317 1.00 53.47
ATOM 2330 CG PRO B 705 -10.713 17.142 -44.308 1.00 53.49
ATOM 2331 CD PRO B 705 -11.394 16.102 -43.457 1.00 53.49
ATOM 2332 N ASN B 706 -7.005 15.018 -44.668 1.00 50.16
ATOM 2333 CA ASN B 706 -5.614 15.255 -44.352 1.00 47.68
ATOM 2334 C ASN B 706 -5.141 16.419 -45.220 1.00 48.60
ATOM 2335 O ASN B 706 -4.817 16.235 -46.394 1.00 47.17
ATOM 2336 CB ASN B 706 -4.798 14.007 -44.679 1.00 46.68
ATOM 2337 CG ASN B 706 -3.336 14.152 -44.307 1.00 47.50
ATOM 2338 OD1 ASN B 706 -2.843 15.264 -44.085 1.00 46.16
ATOM 2339 ND2 ASN B 706 -2.624 13.025 -44.252 1.00 47.14
ATOM 2340 N GLN B 707 -5.089 17.616 -44.654 1.00 48.45
ATOM 2341 CA GLN B 707 -4.663 18.753 -45.448 1.00 50.34
ATOM 2342 C GLN B 707 -3.195 19.132 -45.296 1.00 49.32
ATOM 2343 O GLN B 707 -2.820 20.282 -45.508 1.00 48.81
ATOM 2344 CB GLN B 707 -5.565 19.961 -45.172 1.00 51.33
ATOM 2345 CG GLN B 707 -7.017 19.707 -45.534 1.00 54.04
ATOM 2346 CD GLN B 707 -7.890 20.942 -45.390 1.00 57.85
ATOM 2347 OE1 GLN B 707 -7.874 21.834 -46.244 1.00 59.23
ATOM 2348 NE2 GLN B 707 -8.651 21.007 -44.296 1.00 57.51
ATOM 2349 N ALA B 708 -2.361 18.160 -44.944 1.00 49.01
ATOM 2350 CA ALA B 708 -0.930 18.416 -44.814 1.00 49.28
ATOM 2351 C ALA B 708 -0.402 18.939 -46.153 1.00 50.28
ATOM 2352 O ALA B 708 -0.927 18.609 -47.216 1.00 50.22
ATOM 2353 CB ALA B 708 -0.201 17.134 -44.434 1.00 46.73
ATOM 2354 N GLN B 709 0.635 19.761 -46.102 1.00 52.30
ATOM 2355 CA GLN B 709 1.209 20.305 -47.320 1.00 53.30
ATOM 2356 C GLN B 709 2.521 19.639 -47.662 1.00 54.63
ATOM 2357 O GLN B 709 3.328 19.342 -46.788 1.00 55.25
ATOM 2358 CB GLN B 709 1.438 21.807 -47.173 1.00 53.77
ATOM 2359 CG GLN B 709 0.187 22.623 -47.359 1.00 56.18
ATOM 2360 CD GLN B 709 -0.326 22.555 -48.777 1.00 58.18
ATOM 2361 OE1 GLN B 709 -1.494 22.832 -49.037 1.00 59.37
ATOM 2362 NE2 GLN B 709 0.553 22.197 -49.710 1.00 59.96
ATOM 2363 N LEU B 710 2.734 19.394 -48.943 1.00 56.61
ATOM 2364 CA LEU B 710 3.984 18.793 -49.368 1.00 59.18
ATOM 2365 C LEU B 710 4.565 19.616 -50.508 1.00 59.54
ATOM 2366 O LEU B 710 4.077 19.563 -51.634 1.00 60.05
ATOM 2367 CB LEU B 710 3.788 17.341 -49.826 1.00 58.84
ATOM 2368 CG LEU B 710 5.144 16.673 -50.079 1.00 58.85
ATOM 2369 CD1 LEU B 710 5.941 16.662 -48.780 1.00 56.82
ATOM 2370 CD2 LEU B 710 4.960 15.272 -50.610 1.00 59.31
ATOM 2371 N ARG B 711 5.602 20.385 -50.201 1.00 59.61
ATOM 2372 CA ARG B 711 6.249 21.218 -51.199 1.00 59.44

ATOM 2373 C ARG B 711 7.209 20.387 -52.020 1.00 57.96
ATOM 2374 O ARG B 711 8.038 19.665 -51.487 1.00 56.87
ATOM 2375 CB ARG B 711 7.026 22.352 -50.528 1.00 62.07
ATOM 2376 CG ARG B 711 6.173 23.468 -49.947 1.00 66.77
ATOM 2377 CD ARG B 711 6.166 24.664 -50.880 1.00 70.76
ATOM 2378 NE ARG B 711 5.529 25.830 -50.275 1.00 73.86
ATOM 2379 CZ ARG B 711 5.482 27.030 -50.849 1.00 73.77
ATOM 2380 NH1 ARG B 711 6.038 27.213 -52.039 1.00 71.33
ATOM 2381 NH2 ARG B 711 4.872 28.041 -50.241 1.00 74.12
ATOM 2382 N ILE B 712 7.073 20.472 -53.331 1.00 58.48
ATOM 2383 CA ILE B 712 7.968 19.765 -54.221 1.00 59.27
ATOM 2384 C ILE B 712 8.952 20.858 -54.638 1.00 60.66
ATOM 2385 O ILE B 712 8.601 21.793 -55.355 1.00 60.01
ATOM 2386 CB ILE B 712 7.177 19.162 -55.390 1.00 58.30
ATOM 2387 CG1 ILE B 712 6.266 18.066 -54.826 1.00 57.96
ATOM 2388 CG2 ILE B 712 8.117 18.601 -56.448 1.00 56.69
ATOM 2389 CD1 ILE B 712 5.405 17.380 -55.840 1.00 61.91
ATOM 2390 N LEU B 713 10.178 20.744 -54.139 1.00 60.97
ATOM 2391 CA LEU B 713 11.201 21.748 -54.374 1.00 61.57
ATOM 2392 C LEU B 713 12.091 21.583 -55.583 1.00 62.89
ATOM 2393 O LEU B 713 12.517 20.476 -55.921 1.00 62.63
ATOM 2394 CB LEU B 713 12.093 21.864 -53.141 1.00 60.62
ATOM 2395 CG LEU B 713 11.375 21.861 -51.796 1.00 60.72
ATOM 2396 CD1 LEU B 713 12.345 22.362 -50.739 1.00 60.07
ATOM 2397 CD2 LEU B 713 10.134 22.743 -51.848 1.00 58.84
ATOM 2398 N ALA B 714 12.388 22.713 -56.216 1.00 63.60
ATOM 2399 CA ALA B 714 13.257 22.724 -57.373 1.00 64.47
ATOM 2400 C ALA B 714 14.663 22.544 -56.828 1.00 65.36
ATOM 2401 O ALA B 714 15.049 23.194 -55.857 1.00 64.64
ATOM 2402 CB ALA B 714 13.136 24.052 -58.115 1.00 65.35
ATOM 2403 N GLU B 715 15.409 21.642 -57.451 1.00 66.38
ATOM 2404 CA GLU B 715 16.786 21.337 -57.075 1.00 68.71
ATOM 2405 C GLU B 715 17.570 22.608 -56.764 1.00 69.58
ATOM 2406 O GLU B 715 18.489 22.606 -55.945 1.00 70.53
ATOM 2407 CB GLU B 715 17.451 20.590 -58.233 1.00 71.46
ATOM 2408 CG GLU B 715 18.838 20.031 -57.972 1.00 75.03
ATOM 2409 CD GLU B 715 19.366 19.255 -59.174 1.00 78.03
ATOM 2410 OE1 GLU B 715 20.444 18.627 -59.064 1.00 81.21
ATOM 2411 OE2 GLU B 715 18.699 19.275 -60.234 1.00 78.12
ATOM 2412 N THR B 716 17.178 23.692 -57.422 1.00 69.78
ATOM 2413 CA THR B 716 17.825 24.987 -57.283 1.00 69.47
ATOM 2414 C THR B 716 17.451 25.789 -56.041 1.00 69.52
ATOM 2415 O THR B 716 18.240 26.611 -55.573 1.00 70.64
ATOM 2416 CB THR B 716 17.536 25.866 -58.513 1.00 70.06
ATOM 2417 OG1 THR B 716 18.171 27.138 -58.351 1.00 71.27

ATOM 2418 CG2 THR B 716 16.036 26.076 -58.678 1.00 69.60
ATOM 2419 N GLU B 717 16.253 25.577 -55.511 1.00 68.00
ATOM 2420 CA GLU B 717 15.845 26.321 -54.330 1.00 66.43
ATOM 2421 C GLU B 717 16.699 25.898 -53.135 1.00 66.27
ATOM 2422 O GLU B 717 16.735 26.588 -52.117 1.00 65.77
ATOM 2423 CB GLU B 717 14.363 26.072 -54.032 1.00 67.50
ATOM 2424 CG GLU B 717 13.430 26.254 -55.234 1.00 67.97
ATOM 2425 CD GLU B 717 11.971 25.930 -54.911 1.00 68.95
ATOM 2426 OE1 GLU B 717 11.314 25.253 -55.736 1.00 69.80
ATOM 2427 OE2 GLU B 717 11.479 26.355 -53.843 1.00 67.07
ATOM 2428 N LEU B 718 17.409 24.778 -53.277 1.00 66.24
ATOM 2429 CA LEU B 718 18.240 24.241 -52.197 1.00 67.00
ATOM 2430 C LEU B 718 19.741 24.416 -52.344 1.00 68.38
ATOM 2431 O LEU B 718 20.308 24.173 -53.410 1.00 68.22
ATOM 2432 CB LEU B 718 17.961 22.746 -51.989 1.00 64.67
ATOM 2433 CG LEU B 718 16.592 22.299 -51.473 1.00 64.09
ATOM 2434 CD1 LEU B 718 16.642 20.805 -51.218 1.00 64.50
ATOM 2435 CD2 LEU B 718 16.221 23.038 -50.196 1.00 61.97
ATOM 2436 N ALA B 719 20.376 24.807 -51.240 1.00 69.63
ATOM 2437 CA ALA B 719 21.820 25.008 -51.188 1.00 70.57
ATOM 2438 C ALA B 719 22.409 24.242 -50.006 1.00 71.59
ATOM 2439 O ALA B 719 21.972 24.404 -48.859 1.00 71.07
ATOM 2440 CB ALA B 719 22.152 26.499 -51.062 1.00 69.58
ATOM 2441 N ARG B 720 23.399 23.404 -50.303 1.00 72.39
ATOM 2442 CA ARG B 720 24.083 22.601 -49.296 1.00 73.45
ATOM 2443 C ARG B 720 25.143 23.436 -48.577 1.00 74.60
ATOM 2444 O ARG B 720 25.385 24.593 -48.911 1.00 75.29
ATOM 2445 CB ARG B 720 24.786 21.414 -49.952 1.00 73.03
ATOM 2446 CG ARG B 720 23.902 20.485 -50.756 1.00 74.45
ATOM 2447 CD ARG B 720 23.856 19.106 -50.118 1.00 75.59
ATOM 2448 NE ARG B 720 23.875 18.018 -51.097 1.00 76.81
ATOM 2449 CZ ARG B 720 22.976 17.855 -52.063 1.00 76.86
ATOM 2450 NH1 ARG B 720 21.972 18.714 -52.198 1.00 76.25
ATOM 2451 NH2 ARG B 720 23.074 16.818 -52.886 1.00 77.66
ATOM 2452 N VAL B 721 25.774 22.831 -47.583 1.00 75.37
ATOM 2453 CA VAL B 721 26.835 23.472 -46.824 1.00 75.73
ATOM 2454 C VAL B 721 27.804 22.356 -46.447 1.00 76.50
ATOM 2455 O VAL B 721 28.600 21.912 -47.275 1.00 76.71
ATOM 2456 CB VAL B 721 26.297 24.148 -45.550 1.00 76.20
ATOM 2457 CG1 VAL B 721 27.451 24.684 -44.722 1.00 76.08
ATOM 2458 CG2 VAL B 721 25.358 25.282 -45.925 1.00 75.75
ATOM 2459 N ALA B 722 27.722 21.889 -45.208 1.00 77.05
ATOM 2460 CA ALA B 722 28.584 20.809 -44.751 1.00 76.34
ATOM 2461 C ALA B 722 27.735 19.558 -44.559 1.00 75.78
ATOM 2462 O ALA B 722 26.537 19.548 -44.868 1.00 75.60

ATOM 2463 CB ALA B 722 29.262 21.196 -43.433 1.00 76.05
ATOM 2464 N VAL B 723 28.373 18.507 -44.053 1.00 74.68
ATOM 2465 CA VAL B 723 27.714 17.239 -43.777 1.00 71.94
ATOM 2466 C VAL B 723 27.423 17.159 -42.283 1.00 71.54
ATOM 2467 O VAL B 723 28.310 17.399 -41.461 1.00 71.55
ATOM 2468 CB VAL B 723 28.611 16.058 -44.160 1.00 71.07
ATOM 2469 CG1 VAL B 723 28.020 14.767 -43.629 1.00 70.27
ATOM 2470 CG2 VAL B 723 28.764 15.998 -45.672 1.00 71.21
ATOM 2471 N LEU B 724 26.182 16.836 -41.931 1.00 69.67
ATOM 2472 CA LEU B 724 25.806 16.721 -40.529 1.00 66.81
ATOM 2473 C LEU B 724 26.058 15.300 -40.057 1.00 66.43
ATOM 2474 O LEU B 724 26.094 15.032 -38.859 1.00 68.21
ATOM 2475 CB LEU B 724 24.334 17.080 -40.347 1.00 64.61
ATOM 2476 CG LEU B 724 23.992 18.555 -40.555 1.00 64.25
ATOM 2477 CD1 LEU B 724 22.493 18.740 -40.600 1.00 62.81
ATOM 2478 CD2 LEU B 724 24.593 19.379 -39.431 1.00 63.59
ATOM 2479 N GLY B 725 26.248 14.403 -41.018 1.00 65.74
ATOM 2480 CA GLY B 725 26.484 13.004 -40.723 1.00 65.55
ATOM 2481 C GLY B 725 25.812 12.138 -41.777 1.00 67.20
ATOM 2482 O GLY B 725 24.919 12.602 -42.487 1.00 67.07
ATOM 2483 N SER B 726 26.241 10.884 -41.888 1.00 68.22
ATOM 2484 CA SER B 726 25.668 9.957 -42.860 1.00 69.48
ATOM 2485 C SER B 726 25.632 8.553 -42.275 1.00 70.10
ATOM 2486 O SER B 726 26.012 8.344 -41.126 1.00 71.12
ATOM 2487 CB SER B 726 26.504 9.935 -44.139 1.00 70.71
ATOM 2488 OG SER B 726 27.715 9.214 -43.947 1.00 71.56
ATOM 2489 N GLY B 727 25.186 7.593 -43.079 1.00 71.04
ATOM 2490 CA GLY B 727 25.109 6.217 -42.623 1.00 72.17
ATOM 2491 C GLY B 727 24.190 5.350 -43.469 1.00 72.74
ATOM 2492 O GLY B 727 23.941 5.645 -44.642 1.00 73.49
ATOM 2493 N ALA B 728 23.683 4.280 -42.865 1.00 72.58
ATOM 2494 CA ALA B 728 22.794 3.342 -43.539 1.00 72.96
ATOM 2495 C ALA B 728 21.657 4.049 -44.263 1.00 74.25
ATOM 2496 O ALA B 728 21.285 3.682 -45.381 1.00 73.50
ATOM 2497 CB ALA B 728 22.226 2.361 -42.527 1.00 71.89
ATOM 2498 N PHE B 729 21.110 5.071 -43.618 1.00 76.13
ATOM 2499 CA PHE B 729 20.003 5.825 -44.186 1.00 78.00
ATOM 2500 C PHE B 729 20.488 7.116 -44.823 1.00 78.39
ATOM 2501 O PHE B 729 20.531 8.153 -44.167 1.00 80.61
ATOM 2502 CB PHE B 729 18.980 6.125 -43.091 1.00 78.54
ATOM 2503 CG PHE B 729 18.734 4.958 -42.176 1.00 80.05
ATOM 2504 CD1 PHE B 729 19.552 4.741 -41.067 1.00 80.31
ATOM 2505 CD2 PHE B 729 17.731 4.029 -42.464 1.00 80.12
ATOM 2506 CE1 PHE B 729 19.379 3.613 -40.258 1.00 79.48
ATOM 2507 CE2 PHE B 729 17.551 2.902 -41.666 1.00 79.41

```
ATOM   2508  CZ  PHE B 729      18.378   2.694 -40.561  1.00 80.03
ATOM   2509  N   GLY B 730      20.867   7.040 -46.098  1.00 77.21
ATOM   2510  CA  GLY B 730      21.343   8.209 -46.819  1.00 75.57
ATOM   2511  C   GLY B 730      22.288   9.121 -46.055  1.00 74.55
ATOM   2512  O   GLY B 730      22.876   8.721 -45.051  1.00 74.34
ATOM   2513  N   THR B 731      22.447  10.349 -46.540  1.00 73.71
ATOM   2514  CA  THR B 731      23.322  11.316 -45.887  1.00 72.89
ATOM   2515  C   THR B 731      22.575  12.607 -45.597  1.00 72.69
ATOM   2516  O   THR B 731      21.765  13.069 -46.406  1.00 72.79
ATOM   2517  CB  THR B 731      24.547  11.650 -46.751  1.00 73.00
ATOM   2518  OG1 THR B 731      25.364  10.484 -46.894  1.00 72.99
ATOM   2519  CG2 THR B 731      25.367  12.753 -46.100  1.00 72.78
ATOM   2520  N   VAL B 732      22.854  13.186 -44.434  1.00 72.09
ATOM   2521  CA  VAL B 732      22.204  14.422 -44.025  1.00 71.72
ATOM   2522  C   VAL B 732      23.109  15.616 -44.283  1.00 71.79
ATOM   2523  O   VAL B 732      24.312  15.553 -44.053  1.00 73.24
ATOM   2524  CB  VAL B 732      21.817  14.385 -42.525  1.00 71.31
ATOM   2525  CG1 VAL B 732      21.170  15.704 -42.124  1.00 70.14
ATOM   2526  CG2 VAL B 732      20.858  13.220 -42.256  1.00 69.55
ATOM   2527  N   TYR B 733      22.517  16.703 -44.762  1.00 71.37
ATOM   2528  CA  TYR B 733      23.256  17.915 -45.072  1.00 70.26
ATOM   2529  C   TYR B 733      22.636  19.144 -44.437  1.00 70.40
ATOM   2530  O   TYR B 733      21.423  19.328 -44.475  1.00 69.19
ATOM   2531  CB  TYR B 733      23.280  18.136 -46.581  1.00 71.02
ATOM   2532  CG  TYR B 733      24.205  17.228 -47.350  1.00 72.14
ATOM   2533  CD1 TYR B 733      25.552  17.550 -47.516  1.00 72.40
ATOM   2534  CD2 TYR B 733      23.733  16.051 -47.928  1.00 72.72
ATOM   2535  CE1 TYR B 733      26.403  16.722 -48.244  1.00 72.86
ATOM   2536  CE2 TYR B 733      24.573  15.215 -48.654  1.00 72.43
ATOM   2537  CZ  TYR B 733      25.904  15.556 -48.807  1.00 72.95
ATOM   2538  OH  TYR B 733      26.734  14.728 -49.519  1.00 73.75
ATOM   2539  N   LYS B 734      23.468  19.988 -43.845  1.00 71.52
ATOM   2540  CA  LYS B 734      22.971  21.235 -43.278  1.00 71.70
ATOM   2541  C   LYS B 734      22.836  22.110 -44.526  1.00 70.70
ATOM   2542  O   LYS B 734      23.636  21.981 -45.457  1.00 69.26
ATOM   2543  CB  LYS B 734      24.000  21.843 -42.323  1.00 72.03
ATOM   2544  CG  LYS B 734      23.619  23.219 -41.810  1.00 73.15
ATOM   2545  CD  LYS B 734      24.811  23.927 -41.173  1.00 74.86
ATOM   2546  CE  LYS B 734      24.469  25.371 -40.815  1.00 75.25
ATOM   2547  NZ  LYS B 734      25.609  26.084 -40.177  1.00 75.36
ATOM   2548  N   GLY B 735      21.836  22.983 -44.570  1.00 69.60
ATOM   2549  CA  GLY B 735      21.694  23.804 -45.757  1.00 70.34
ATOM   2550  C   GLY B 735      20.674  24.921 -45.717  1.00 70.22
ATOM   2551  O   GLY B 735      20.003  25.146 -44.709  1.00 70.41
ATOM   2552  N   ILE B 736      20.559  25.626 -46.835  1.00 70.46
```

```
ATOM  2553  CA  ILE B 736     19.619  26.730 -46.932  1.00 71.88
ATOM  2554  C   ILE B 736     18.619  26.490 -48.053  1.00 70.97
ATOM  2555  O   ILE B 736     18.988  26.084 -49.158  1.00 70.48
ATOM  2556  CB  ILE B 736     20.344  28.065 -47.216  1.00 73.37
ATOM  2557  CG1 ILE B 736     21.503  28.253 -46.232  1.00 75.08
ATOM  2558  CG2 ILE B 736     19.359  29.225 -47.099  1.00 72.22
ATOM  2559  CD1 ILE B 736     22.363  29.482 -46.523  1.00 77.81
ATOM  2560  N   TRP B 737     17.349  26.734 -47.756  1.00 69.75
ATOM  2561  CA  TRP B 737     16.301  26.571 -48.746  1.00 69.68
ATOM  2562  C   TRP B 737     15.679  27.924 -49.044  1.00 71.04
ATOM  2563  O   TRP B 737     15.167  28.593 -48.142  1.00 70.73
ATOM  2564  CB  TRP B 737     15.219  25.612 -48.247  1.00 67.06
ATOM  2565  CG  TRP B 737     13.973  25.642 -49.085  1.00 63.60
ATOM  2566  CD1 TRP B 737     13.900  25.681 -50.449  1.00 62.26
ATOM  2567  CD2 TRP B 737     12.623  25.615 -48.614  1.00 62.62
ATOM  2568  NE1 TRP B 737     12.589  25.683 -50.857  1.00 61.65
ATOM  2569  CE2 TRP B 737     11.783  25.641 -49.752  1.00 61.65
ATOM  2570  CE3 TRP B 737     12.041  25.567 -47.342  1.00 62.03
ATOM  2571  CZ2 TRP B 737     10.393  25.621 -49.658  1.00 61.01
ATOM  2572  CZ3 TRP B 737     10.657  25.545 -47.246  1.00 63.21
ATOM  2573  CH2 TRP B 737      9.847  25.573 -48.402  1.00 62.84
ATOM  2574  N   VAL B 738     15.727  28.320 -50.313  1.00 71.93
ATOM  2575  CA  VAL B 738     15.162  29.590 -50.738  1.00 72.89
ATOM  2576  C   VAL B 738     13.895  29.317 -51.539  1.00 74.11
ATOM  2577  O   VAL B 738     13.960  29.000 -52.722  1.00 74.51
ATOM  2578  CB  VAL B 738     16.155  30.357 -51.614  1.00 73.24
ATOM  2579  CG1 VAL B 738     15.753  31.811 -51.677  1.00 72.41
ATOM  2580  CG2 VAL B 738     17.573  30.189 -51.067  1.00 71.96
ATOM  2581  N   PRO B 739     12.723  29.441 -50.898  1.00 75.71
ATOM  2582  CA  PRO B 739     11.408  29.212 -51.504  1.00 78.23
ATOM  2583  C   PRO B 739     11.246  29.754 -52.922  1.00 80.64
ATOM  2584  O   PRO B 739     11.912  30.716 -53.309  1.00 80.64
ATOM  2585  CB  PRO B 739     10.462  29.882 -50.518  1.00 77.56
ATOM  2586  CG  PRO B 739     11.135  29.618 -49.210  1.00 77.83
ATOM  2587  CD  PRO B 739     12.574  29.957 -49.527  1.00 76.20
ATOM  2588  N   ALA B 740     10.348  29.128 -53.682  1.00 83.02
ATOM  2589  CA  ALA B 740     10.077  29.521 -55.062  1.00 84.99
ATOM  2590  C   ALA B 740      9.540  30.948 -55.142  1.00 86.49
ATOM  2591  O   ALA B 740      8.328  31.168 -55.063  1.00 87.30
ATOM  2592  CB  ALA B 740      9.080  28.554 -55.695  1.00 84.35
ATOM  2593  N   GLY B 741     10.449  31.912 -55.293  1.00 87.21
ATOM  2594  CA  GLY B 741     10.048  33.306 -55.390  1.00 88.15
ATOM  2595  C   GLY B 741     10.039  34.051 -54.069  1.00 88.91
ATOM  2596  O   GLY B 741      9.134  34.841 -53.796  1.00 89.07
ATOM  2597  N   GLU B 742     11.051  33.804 -53.245  1.00 89.01
```

```
ATOM   2598  CA  GLU B 742      11.146  34.460 -51.949  1.00 89.25
ATOM   2599  C   GLU B 742      12.605  34.733 -51.597  1.00 89.18
ATOM   2600  O   GLU B 742      13.514  34.121 -52.163  1.00 87.36
ATOM   2601  CB  GLU B 742      10.486  33.592 -50.874  1.00 89.33
ATOM   2602  CG  GLU B 742       9.030  33.270 -51.166  1.00 89.86
ATOM   2603  CD  GLU B 742       8.394  32.409 -50.096  1.00 91.41
ATOM   2604  OE1 GLU B 742       7.217  32.022 -50.259  1.00 92.46
ATOM   2605  OE2 GLU B 742       9.068  32.116 -49.089  1.00 91.98
ATOM   2606  N   ALA B 743      12.818  35.659 -50.664  1.00 89.63
ATOM   2607  CA  ALA B 743      14.163  36.037 -50.241  1.00 89.61
ATOM   2608  C   ALA B 743      14.626  35.259 -49.016  1.00 89.33
ATOM   2609  O   ALA B 743      15.813  34.951 -48.884  1.00 89.32
ATOM   2610  CB  ALA B 743      14.219  37.538 -49.956  1.00 88.93
ATOM   2611  N   VAL B 744      13.692  34.944 -48.122  1.00 88.36
ATOM   2612  CA  VAL B 744      14.016  34.203 -46.902  1.00 86.73
ATOM   2613  C   VAL B 744      14.987  33.060 -47.185  1.00 85.49
ATOM   2614  O   VAL B 744      14.800  32.293 -48.129  1.00 86.20
ATOM   2615  CB  VAL B 744      12.744  33.615 -46.239  1.00 86.40
ATOM   2616  CG1 VAL B 744      11.827  34.737 -45.777  1.00 86.46
ATOM   2617  CG2 VAL B 744      12.018  32.709 -47.217  1.00 86.17
ATOM   2618  N   ALA B 745      16.033  32.959 -46.373  1.00 83.22
ATOM   2619  CA  ALA B 745      17.020  31.901 -46.537  1.00 80.32
ATOM   2620  C   ALA B 745      16.858  30.887 -45.402  1.00 78.54
ATOM   2621  O   ALA B 745      17.722  30.780 -44.537  1.00 77.78
ATOM   2622  CB  ALA B 745      18.426  32.497 -46.528  1.00 79.74
ATOM   2623  N   ILE B 746      15.742  30.154 -45.415  1.00 76.18
ATOM   2624  CA  ILE B 746      15.427  29.144 -44.394  1.00 73.00
ATOM   2625  C   ILE B 746      16.506  28.085 -44.148  1.00 70.60
ATOM   2626  O   ILE B 746      16.926  27.379 -45.068  1.00 70.94
ATOM   2627  CB  ILE B 746      14.133  28.384 -44.740  1.00 73.31
ATOM   2628  CG1 ILE B 746      12.939  29.338 -44.735  1.00 74.65
ATOM   2629  CG2 ILE B 746      13.906  27.271 -43.733  1.00 73.54
ATOM   2630  CD1 ILE B 746      11.630  28.690 -45.169  1.00 74.90
ATOM   2631  N   PRO B 747      16.963  27.959 -42.890  1.00 68.46
ATOM   2632  CA  PRO B 747      17.991  26.973 -42.542  1.00 66.18
ATOM   2633  C   PRO B 747      17.322  25.609 -42.442  1.00 63.94
ATOM   2634  O   PRO B 747      16.327  25.441 -41.727  1.00 62.47
ATOM   2635  CB  PRO B 747      18.499  27.475 -41.198  1.00 65.24
ATOM   2636  CG  PRO B 747      17.258  28.014 -40.581  1.00 65.83
ATOM   2637  CD  PRO B 747      16.625  28.788 -41.718  1.00 67.44
ATOM   2638  N   VAL B 748      17.864  24.638 -43.162  1.00 61.19
ATOM   2639  CA  VAL B 748      17.273  23.316 -43.161  1.00 60.40
ATOM   2640  C   VAL B 748      18.273  22.179 -43.190  1.00 60.05
ATOM   2641  O   VAL B 748      19.484  22.383 -43.273  1.00 59.27
ATOM   2642  CB  VAL B 748      16.346  23.121 -44.382  1.00 60.82
```

ATOM 2643 CG1 VAL B 748 15.250 24.166 -44.384 1.00 60.94
ATOM 2644 CG2 VAL B 748 17.159 23.192 -45.662 1.00 58.19
ATOM 2645 N ALA B 749 17.726 20.973 -43.110 1.00 59.07
ATOM 2646 CA ALA B 749 18.503 19.757 -43.177 1.00 59.25
ATOM 2647 C ALA B 749 18.025 19.161 -44.489 1.00 60.46
ATOM 2648 O ALA B 749 16.899 19.422 -44.910 1.00 61.58
ATOM 2649 CB ALA B 749 18.159 18.837 -42.019 1.00 57.97
ATOM 2650 N ILE B 750 18.881 18.388 -45.144 1.00 60.55
ATOM 2651 CA ILE B 750 18.536 17.762 -46.407 1.00 59.69
ATOM 2652 C ILE B 750 19.113 16.364 -46.376 1.00 60.35
ATOM 2653 O ILE B 750 20.304 16.182 -46.120 1.00 59.91
ATOM 2654 CB ILE B 750 19.152 18.519 -47.593 1.00 60.90
ATOM 2655 CG1 ILE B 750 18.855 20.014 -47.470 1.00 61.45
ATOM 2656 CG2 ILE B 750 18.593 17.976 -48.898 1.00 61.29
ATOM 2657 CD1 ILE B 750 19.552 20.868 -48.512 1.00 62.03
ATOM 2658 N LYS B 751 18.272 15.373 -46.629 1.00 60.64
ATOM 2659 CA LYS B 751 18.736 14.003 -46.608 1.00 61.71
ATOM 2660 C LYS B 751 18.568 13.371 -47.970 1.00 64.10
ATOM 2661 O LYS B 751 17.569 13.593 -48.652 1.00 63.74
ATOM 2662 CB LYS B 751 17.962 13.216 -45.557 1.00 60.11
ATOM 2663 CG LYS B 751 18.422 11.788 -45.379 1.00 58.61
ATOM 2664 CD LYS B 751 17.930 11.241 -44.049 1.00 58.06
ATOM 2665 CE LYS B 751 18.424 9.840 -43.818 1.00 56.70
ATOM 2666 NZ LYS B 751 18.112 9.366 -42.448 1.00 57.25
ATOM 2667 N ILE B 752 19.562 12.590 -48.367 1.00 67.30
ATOM 2668 CA ILE B 752 19.532 11.909 -49.650 1.00 70.25
ATOM 2669 C ILE B 752 19.714 10.425 -49.393 1.00 71.94
ATOM 2670 O ILE B 752 20.740 10.013 -48.867 1.00 73.06
ATOM 2671 CB ILE B 752 20.666 12.407 -50.556 1.00 70.74
ATOM 2672 CG1 ILE B 752 20.578 13.930 -50.705 1.00 70.64
ATOM 2673 CG2 ILE B 752 20.578 11.721 -51.912 1.00 71.95
ATOM 2674 CD1 ILE B 752 21.674 14.538 -51.555 1.00 69.52
ATOM 2675 N ALA B 753 18.723 9.623 -49.760 1.00 74.71
ATOM 2676 CA ALA B 753 18.799 8.185 -49.536 1.00 78.36
ATOM 2677 C ALA B 753 19.570 7.481 -50.639 1.00 81.19
ATOM 2678 O ALA B 753 19.369 7.757 -51.821 1.00 81.29
ATOM 2679 CB ALA B 753 17.399 7.601 -49.423 1.00 77.47
ATOM 2680 N VAL B 754 20.453 6.570 -50.238 1.00 85.07
ATOM 2681 CA VAL B 754 21.281 5.798 -51.170 1.00 88.42
ATOM 2682 C VAL B 754 20.468 5.271 -52.358 1.00 90.41
ATOM 2683 O VAL B 754 19.817 4.229 -52.260 1.00 91.29
ATOM 2684 CB VAL B 754 21.940 4.581 -50.459 1.00 88.45
ATOM 2685 CG1 VAL B 754 23.015 3.969 -51.357 1.00 86.93
ATOM 2686 CG2 VAL B 754 22.519 5.009 -49.108 1.00 88.93
ATOM 2687 N ALA B 755 20.517 5.991 -53.477 1.00 91.96

ATOM 2688 CA ALA B 755 19.789 5.605 -54.684 1.00 93.14
ATOM 2689 CB ALA B 755 20.303 6.403 -55.878 1.00 92.70
ATOM 2690 C ALA B 755 19.890 4.104 -54.975 1.00 94.28
ATOM 2691 OT1 ALA B 755 18.831 3.482 -55.224 1.00 94.26
ATOM 2692 OT2 ALA B 755 21.023 3.569 -54.962 1.00 94.42
ATOM 2693 N ALA B 761 9.723 1.143 -56.947 1.00 87.14
ATOM 2694 CA ALA B 761 10.011 1.599 -55.557 1.00 87.01
ATOM 2695 C ALA B 761 9.596 3.053 -55.300 1.00 87.49
ATOM 2696 O ALA B 761 9.028 3.358 -54.254 1.00 88.29
ATOM 2697 CB ALA B 761 11.492 1.420 -55.252 1.00 86.17
ATOM 2698 N ASN B 762 9.879 3.946 -56.245 1.00 87.30
ATOM 2699 CA ASN B 762 9.532 5.358 -56.091 1.00 86.68
ATOM 2700 C ASN B 762 8.123 5.587 -55.563 1.00 85.76
ATOM 2701 O ASN B 762 7.796 6.676 -55.095 1.00 85.55
ATOM 2702 CB ASN B 762 9.711 6.095 -57.417 1.00 87.83
ATOM 2703 CG ASN B 762 11.145 6.515 -57.652 1.00 88.91
ATOM 2704 OD1 ASN B 762 12.065 5.696 -57.587 1.00 88.14
ATOM 2705 ND2 ASN B 762 11.347 7.800 -57.923 1.00 89.08
ATOM 2706 N VAL B 763 7.288 4.559 -55.645 1.00 84.95
ATOM 2707 CA VAL B 763 5.919 4.652 -55.152 1.00 83.59
ATOM 2708 C VAL B 763 5.981 4.500 -53.634 1.00 82.82
ATOM 2709 O VAL B 763 5.380 5.277 -52.891 1.00 82.67
ATOM 2710 CB VAL B 763 5.039 3.517 -55.713 1.00 83.22
ATOM 2711 CG1 VAL B 763 3.574 3.913 -55.639 1.00 83.32
ATOM 2712 CG2 VAL B 763 5.452 3.190 -57.134 1.00 83.28
ATOM 2713 N ALA B 764 6.723 3.485 -53.192 1.00 81.06
ATOM 2714 CA ALA B 764 6.899 3.188 -51.774 1.00 79.39
ATOM 2715 C ALA B 764 7.374 4.428 -51.024 1.00 77.74
ATOM 2716 O ALA B 764 7.068 4.616 -49.841 1.00 77.59
ATOM 2717 CB ALA B 764 7.911 2.048 -51.601 1.00 78.81
ATOM 2718 N PHE B 765 8.124 5.269 -51.727 1.00 75.13
ATOM 2719 CA PHE B 765 8.653 6.497 -51.156 1.00 72.04
ATOM 2720 C PHE B 765 7.617 7.621 -51.141 1.00 69.21
ATOM 2721 O PHE B 765 7.398 8.271 -50.120 1.00 67.19
ATOM 2722 CB PHE B 765 9.890 6.937 -51.939 1.00 72.95
ATOM 2723 CG PHE B 765 10.256 8.364 -51.716 1.00 74.51
ATOM 2724 CD1 PHE B 765 9.604 9.378 -52.416 1.00 76.66
ATOM 2725 CD2 PHE B 765 11.187 8.708 -50.749 1.00 74.99
ATOM 2726 CE1 PHE B 765 9.868 10.717 -52.152 1.00 76.83
ATOM 2727 CE2 PHE B 765 11.460 10.042 -50.474 1.00 76.87
ATOM 2728 CZ PHE B 765 10.797 11.053 -51.177 1.00 77.47
ATOM 2729 N MET B 766 6.989 7.858 -52.281 1.00 67.05
ATOM 2730 CA MET B 766 5.990 8.903 -52.362 1.00 66.91
ATOM 2731 C MET B 766 4.876 8.664 -51.351 1.00 66.11
ATOM 2732 O MET B 766 4.201 9.598 -50.924 1.00 66.81

```
ATOM   2733  CB  MET B 766      5.412   8.975 -53.778  1.00 68.18
ATOM   2734  CG  MET B 766      6.425   9.399 -54.826  1.00 68.28
ATOM   2735  SD  MET B 766      7.326  10.874 -54.318  1.00 68.93
ATOM   2736  CE  MET B 766      6.095  12.100 -54.463  1.00 67.19
ATOM   2737  N   ASP B 767      4.678   7.412 -50.966  1.00 64.47
ATOM   2738  CA  ASP B 767      3.642   7.109 -49.997  1.00 63.79
ATOM   2739  C   ASP B 767      4.142   7.370 -48.587  1.00 61.82
ATOM   2740  O   ASP B 767      3.420   7.922 -47.761  1.00 61.10
ATOM   2741  CB  ASP B 767      3.186   5.660 -50.146  1.00 67.06
ATOM   2742  CG  ASP B 767      2.150   5.490 -51.246  1.00 70.14
ATOM   2743  OD1 ASP B 767      1.000   5.939 -51.059  1.00 71.60
ATOM   2744  OD2 ASP B 767      2.484   4.917 -52.304  1.00 73.46
ATOM   2745  N   GLU B 768      5.385   6.984 -48.320  1.00 60.15
ATOM   2746  CA  GLU B 768      5.978   7.194 -47.008  1.00 58.81
ATOM   2747  C   GLU B 768      6.184   8.689 -46.770  1.00 57.14
ATOM   2748  O   GLU B 768      6.001   9.184 -45.654  1.00 54.76
ATOM   2749  CB  GLU B 768      7.319   6.459 -46.906  1.00 61.07
ATOM   2750  CG  GLU B 768      7.904   6.444 -45.495  1.00 64.70
ATOM   2751  CD  GLU B 768      7.060   5.642 -44.506  1.00 66.61
ATOM   2752  OE1 GLU B 768      7.238   5.825 -43.283  1.00 68.31
ATOM   2753  OE2 GLU B 768      6.227   4.823 -44.948  1.00 66.65
ATOM   2754  N   ALA B 769      6.553   9.405 -47.829  1.00 55.28
ATOM   2755  CA  ALA B 769      6.773  10.841 -47.736  1.00 54.43
ATOM   2756  C   ALA B 769      5.491  11.555 -47.326  1.00 54.12
ATOM   2757  O   ALA B 769      5.535  12.625 -46.717  1.00 56.14
ATOM   2758  CB  ALA B 769      7.274  11.385 -49.065  1.00 53.75
ATOM   2759  N   LEU B 770      4.346  10.970 -47.657  1.00 52.05
ATOM   2760  CA  LEU B 770      3.077  11.576 -47.287  1.00 51.69
ATOM   2761  C   LEU B 770      2.921  11.494 -45.774  1.00 51.45
ATOM   2762  O   LEU B 770      2.470  12.440 -45.125  1.00 52.01
ATOM   2763  CB  LEU B 770      1.910  10.864 -47.991  1.00 52.43
ATOM   2764  CG  LEU B 770      0.511  11.393 -47.636  1.00 53.86
ATOM   2765  CD1 LEU B 770     -0.417  11.306 -48.839  1.00 54.92
ATOM   2766  CD2 LEU B 770     -0.041  10.608 -46.450  1.00 52.30
ATOM   2767  N   ILE B 771      3.307  10.357 -45.211  1.00 50.57
ATOM   2768  CA  ILE B 771      3.216  10.175 -43.775  1.00 50.50
ATOM   2769  C   ILE B 771      4.203  11.092 -43.060  1.00 50.19
ATOM   2770  O   ILE B 771      3.883  11.700 -42.047  1.00 51.29
ATOM   2771  CB  ILE B 771      3.511   8.726 -43.377  1.00 50.14
ATOM   2772  CG1 ILE B 771      2.554   7.778 -44.105  1.00 51.79
ATOM   2773  CG2 ILE B 771      3.340   8.569 -41.885  1.00 48.70
ATOM   2774  CD1 ILE B 771      1.078   8.018 -43.775  1.00 51.92
ATOM   2775  N   MET B 772      5.409  11.197 -43.587  1.00 50.96
ATOM   2776  CA  MET B 772      6.395  12.056 -42.962  1.00 52.41
ATOM   2777  C   MET B 772      5.918  13.499 -42.960  1.00 53.45
```

```
ATOM   2778  O   MET B 772      6.222  14.262 -42.053  1.00 56.84
ATOM   2779  CB  MET B 772      7.727  11.960 -43.698  1.00 51.86
ATOM   2780  CG  MET B 772      8.323  10.581 -43.694  1.00 51.45
ATOM   2781  SD  MET B 772      9.869  10.566 -44.572  1.00 54.95
ATOM   2782  CE  MET B 772     10.510   8.976 -44.043  1.00 57.12
ATOM   2783  N   ALA B 773      5.156  13.875 -43.971  1.00 53.69
ATOM   2784  CA  ALA B 773      4.680  15.240 -44.048  1.00 53.73
ATOM   2785  C   ALA B 773      3.350  15.455 -43.331  1.00 53.40
ATOM   2786  O   ALA B 773      2.955  16.588 -43.076  1.00 54.15
ATOM   2787  CB  ALA B 773      4.567  15.651 -45.512  1.00 55.36
ATOM   2788  N   SER B 774      2.653  14.380 -42.995  1.00 53.47
ATOM   2789  CA  SER B 774      1.370  14.536 -42.321  1.00 54.15
ATOM   2790  C   SER B 774      1.499  14.673 -40.805  1.00 54.10
ATOM   2791  O   SER B 774      0.512  14.933 -40.126  1.00 55.42
ATOM   2792  CB  SER B 774      0.457  13.352 -42.637  1.00 54.46
ATOM   2793  OG  SER B 774      0.363  13.121 -44.027  1.00 57.39
ATOM   2794  N   MET B 775      2.705  14.509 -40.275  1.00 53.87
ATOM   2795  CA  MET B 775      2.924  14.594 -38.830  1.00 54.89
ATOM   2796  C   MET B 775      2.843  15.992 -38.190  1.00 54.27
ATOM   2797  O   MET B 775      3.665  16.858 -38.460  1.00 54.83
ATOM   2798  CB  MET B 775      4.265  13.946 -38.496  1.00 55.60
ATOM   2799  CG  MET B 775      4.357  12.524 -39.000  1.00 57.72
ATOM   2800  SD  MET B 775      2.881  11.559 -38.576  1.00 63.74
ATOM   2801  CE  MET B 775      3.577  10.256 -37.670  1.00 57.19
ATOM   2802  N   ASP B 776      1.853  16.194 -37.323  1.00 54.06
ATOM   2803  CA  ASP B 776      1.660  17.475 -36.645  1.00 53.45
ATOM   2804  C   ASP B 776      1.627  17.322 -35.119  1.00 52.22
ATOM   2805  O   ASP B 776      0.565  17.293 -34.493  1.00 51.95
ATOM   2806  CB  ASP B 776      0.369  18.136 -37.133  1.00 55.05
ATOM   2807  CG  ASP B 776      0.193  19.550 -36.595  1.00 57.95
ATOM   2808  OD1 ASP B 776      1.211  20.168 -36.195  1.00 56.53
ATOM   2809  OD2 ASP B 776     -0.961  20.046 -36.589  1.00 56.88
ATOM   2810  N   HIS B 777      2.810  17.234 -34.529  1.00 50.34
ATOM   2811  CA  HIS B 777      2.948  17.073 -33.094  1.00 47.37
ATOM   2812  C   HIS B 777      4.238  17.764 -32.718  1.00 47.49
ATOM   2813  O   HIS B 777      5.264  17.580 -33.374  1.00 45.96
ATOM   2814  CB  HIS B 777      3.009  15.589 -32.737  1.00 45.58
ATOM   2815  CG  HIS B 777      3.097  15.319 -31.268  1.00 45.70
ATOM   2816  ND1 HIS B 777      4.262  15.481 -30.549  1.00 46.20
ATOM   2817  CD2 HIS B 777      2.168  14.882 -30.386  1.00 44.55
ATOM   2818  CE1 HIS B 777      4.048  15.154 -29.287  1.00 44.22
ATOM   2819  NE2 HIS B 777      2.785  14.786 -29.162  1.00 46.79
ATOM   2820  N   PRO B 778      4.204  18.572 -31.649  1.00 48.64
ATOM   2821  CA  PRO B 778      5.382  19.308 -31.183  1.00 48.65
ATOM   2822  C   PRO B 778      6.636  18.467 -30.938  1.00 48.69
```

```
ATOM   2823  O   PRO B 778      7.755  18.986 -30.992  1.00 50.23
ATOM   2824  CB  PRO B 778      4.871  20.020 -29.924  1.00 48.43
ATOM   2825  CG  PRO B 778      3.796  19.118 -29.435  1.00 48.56
ATOM   2826  CD  PRO B 778      3.089  18.707 -30.694  1.00 47.48
ATOM   2827  N   HIS B 779      6.479  17.169 -30.708  1.00 47.19
ATOM   2828  CA  HIS B 779      7.666  16.366 -30.468  1.00 46.69
ATOM   2829  C   HIS B 779      8.062  15.405 -31.589  1.00 46.92
ATOM   2830  O   HIS B 779      8.806  14.438 -31.387  1.00 45.42
ATOM   2831  CB  HIS B 779      7.543  15.680 -29.108  1.00 43.27
ATOM   2832  CG  HIS B 779      7.436  16.657 -27.979  1.00 42.66
ATOM   2833  ND1 HIS B 779      8.325  17.699 -27.821  1.00 41.28
ATOM   2834  CD2 HIS B 779      6.504  16.808 -27.010  1.00 42.33
ATOM   2835  CE1 HIS B 779      7.940  18.453 -26.808  1.00 42.15
ATOM   2836  NE2 HIS B 779      6.837  17.935 -26.298  1.00 39.93
ATOM   2837  N   LEU B 780      7.583  15.711 -32.788  1.00 46.23
ATOM   2838  CA  LEU B 780      7.920  14.935 -33.968  1.00 46.87
ATOM   2839  C   LEU B 780      8.316  15.921 -35.056  1.00 47.73
ATOM   2840  O   LEU B 780      7.772  17.024 -35.145  1.00 48.06
ATOM   2841  CB  LEU B 780      6.730  14.107 -34.436  1.00 45.91
ATOM   2842  CG  LEU B 780      6.235  12.985 -33.527  1.00 47.10
ATOM   2843  CD1 LEU B 780      5.096  12.287 -34.244  1.00 48.53
ATOM   2844  CD2 LEU B 780      7.349  11.987 -33.216  1.00 46.79
ATOM   2845  N   VAL B 781      9.277  15.540 -35.878  1.00 48.83
ATOM   2846  CA  VAL B 781      9.691  16.432 -36.944  1.00 51.89
ATOM   2847  C   VAL B 781      8.710  16.336 -38.104  1.00 53.37
ATOM   2848  O   VAL B 781      7.995  15.349 -38.258  1.00 52.89
ATOM   2849  CB  VAL B 781     11.109  16.094 -37.444  1.00 50.59
ATOM   2850  CG1 VAL B 781     12.078  16.089 -36.266  1.00 49.98
ATOM   2851  CG2 VAL B 781     11.107  14.757 -38.152  1.00 48.87
ATOM   2852  N   ARG B 782      8.675  17.382 -38.914  1.00 56.80
ATOM   2853  CA  ARG B 782      7.793  17.423 -40.070  1.00 59.13
ATOM   2854  C   ARG B 782      8.643  17.636 -41.316  1.00 58.23
ATOM   2855  O   ARG B 782      9.646  18.364 -41.293  1.00 57.16
ATOM   2856  CB  ARG B 782      6.784  18.562 -39.923  1.00 61.42
ATOM   2857  CG  ARG B 782      5.654  18.537 -40.920  1.00 66.10
ATOM   2858  CD  ARG B 782      4.579  19.529 -40.496  1.00 72.64
ATOM   2859  NE  ARG B 782      3.401  19.499 -41.364  1.00 77.10
ATOM   2860  CZ  ARG B 782      2.293  20.207 -41.147  1.00 78.91
ATOM   2861  NH1 ARG B 782      2.205  21.003 -40.085  1.00 78.69
ATOM   2862  NH2 ARG B 782      1.273  20.129 -41.997  1.00 80.27
ATOM   2863  N   LEU B 783      8.247  16.980 -42.397  1.00 56.30
ATOM   2864  CA  LEU B 783      8.958  17.102 -43.654  1.00 55.96
ATOM   2865  C   LEU B 783      8.383  18.309 -44.374  1.00 54.57
ATOM   2866  O   LEU B 783      7.175  18.392 -44.573  1.00 56.01
ATOM   2867  CB  LEU B 783      8.745  15.839 -44.486  1.00 57.21
```

ATOM 2868 CG LEU B 783 9.516 15.702 -45.795 1.00 55.26
ATOM 2869 CD1 LEU B 783 11.009 15.669 -45.514 1.00 56.03
ATOM 2870 CD2 LEU B 783 9.080 14.436 -46.485 1.00 55.49
ATOM 2871 N LEU B 784 9.242 19.250 -44.747 1.00 54.51
ATOM 2872 CA LEU B 784 8.788 20.450 -45.444 1.00 54.07
ATOM 2873 C LEU B 784 8.526 20.132 -46.903 1.00 52.39
ATOM 2874 O LEU B 784 7.471 20.466 -47.443 1.00 52.32
ATOM 2875 CB LEU B 784 9.832 21.564 -45.340 1.00 54.48
ATOM 2876 CG LEU B 784 10.072 22.091 -43.920 1.00 57.09
ATOM 2877 CD1 LEU B 784 11.245 23.059 -43.919 1.00 57.21
ATOM 2878 CD2 LEU B 784 8.810 22.765 -43.393 1.00 56.32
ATOM 2879 N GLY B 785 9.488 19.470 -47.535 1.00 50.88
ATOM 2880 CA GLY B 785 9.325 19.128 -48.931 1.00 48.30
ATOM 2881 C GLY B 785 10.255 18.057 -49.460 1.00 48.59
ATOM 2882 O GLY B 785 11.104 17.513 -48.755 1.00 46.94
ATOM 2883 N VAL B 786 10.077 17.750 -50.733 1.00 48.89
ATOM 2884 CA VAL B 786 10.891 16.755 -51.381 1.00 49.74
ATOM 2885 C VAL B 786 11.370 17.317 -52.707 1.00 51.57
ATOM 2886 O VAL B 786 10.638 18.059 -53.385 1.00 50.67
ATOM 2887 CB VAL B 786 10.083 15.468 -51.640 1.00 50.26
ATOM 2888 CG1 VAL B 786 10.931 14.473 -52.414 1.00 50.36
ATOM 2889 CG2 VAL B 786 9.638 14.858 -50.320 1.00 49.86
ATOM 2890 N CYS B 787 12.609 16.983 -53.058 1.00 50.94
ATOM 2891 CA CYS B 787 13.187 17.414 -54.316 1.00 51.41
ATOM 2892 C CYS B 787 13.398 16.134 -55.113 1.00 51.83
ATOM 2893 O CYS B 787 14.017 15.193 -54.627 1.00 51.13
ATOM 2894 CB CYS B 787 14.515 18.135 -54.089 1.00 52.49
ATOM 2895 SG CYS B 787 15.263 18.700 -55.644 1.00 57.81
ATOM 2896 N LEU B 788 12.891 16.105 -56.339 1.00 54.13
ATOM 2897 CA LEU B 788 12.975 14.915 -57.173 1.00 57.19
ATOM 2898 C LEU B 788 14.242 14.704 -57.992 1.00 61.05
ATOM 2899 O LEU B 788 14.481 13.599 -58.479 1.00 61.41
ATOM 2900 CB LEU B 788 11.751 14.864 -58.089 1.00 55.35
ATOM 2901 CG LEU B 788 10.426 14.802 -57.311 1.00 56.39
ATOM 2902 CD1 LEU B 788 9.251 14.950 -58.250 1.00 55.47
ATOM 2903 CD2 LEU B 788 10.334 13.487 -56.548 1.00 55.46
ATOM 2904 N SER B 789 15.066 15.737 -58.146 1.00 64.33
ATOM 2905 CA SER B 789 16.285 15.582 -58.938 1.00 66.33
ATOM 2906 C SER B 789 17.520 16.071 -58.192 1.00 66.73
ATOM 2907 O SER B 789 17.424 16.955 -57.336 1.00 66.88
ATOM 2908 CB SER B 789 16.141 16.337 -60.264 1.00 67.97
ATOM 2909 OG SER B 789 17.099 15.892 -61.214 1.00 72.18
ATOM 2910 N PRO B 790 18.697 15.474 -58.477 1.00 67.24
ATOM 2911 CA PRO B 790 18.941 14.388 -59.439 1.00 66.95
ATOM 2912 C PRO B 790 18.245 13.123 -58.965 1.00 67.17

```
ATOM   2913  O   PRO B 790      17.782  12.298 -59.757  1.00 66.12
ATOM   2914  CB  PRO B 790      20.454  14.242 -59.407  1.00 66.69
ATOM   2915  CG  PRO B 790      20.768  14.555 -57.969  1.00 66.95
ATOM   2916  CD  PRO B 790      19.933  15.791 -57.739  1.00 66.62
ATOM   2917  N   THR B 791      18.209  12.987 -57.646  1.00 66.82
ATOM   2918  CA  THR B 791      17.565  11.869 -56.986  1.00 66.98
ATOM   2919  C   THR B 791      16.862  12.492 -55.791  1.00 65.80
ATOM   2920  O   THR B 791      17.173  13.617 -55.392  1.00 64.64
ATOM   2921  CB  THR B 791      18.583  10.805 -56.503  1.00 69.05
ATOM   2922  OG1 THR B 791      19.435  11.370 -55.496  1.00 69.07
ATOM   2923  CG2 THR B 791      19.431  10.306 -57.679  1.00 69.29
ATOM   2924  N   ILE B 792      15.920  11.748 -55.229  1.00 64.46
ATOM   2925  CA  ILE B 792      15.117  12.198 -54.103  1.00 62.56
ATOM   2926  C   ILE B 792      15.841  12.710 -52.871  1.00 61.32
ATOM   2927  O   ILE B 792      16.659  12.011 -52.283  1.00 62.26
ATOM   2928  CB  ILE B 792      14.152  11.093 -53.677  1.00 60.97
ATOM   2929  CG1 ILE B 792      13.035  10.988 -54.710  1.00 61.00
ATOM   2930  CG2 ILE B 792      13.616  11.383 -52.311  1.00 58.92
ATOM   2931  CD1 ILE B 792      12.063   9.871 -54.469  1.00 65.86
ATOM   2932  N   GLN B 793      15.510  13.938 -52.483  1.00 60.22
ATOM   2933  CA  GLN B 793      16.103  14.566 -51.310  1.00 60.54
ATOM   2934  C   GLN B 793      14.994  14.972 -50.352  1.00 59.77
ATOM   2935  O   GLN B 793      13.964  15.522 -50.766  1.00 59.02
ATOM   2936  CB  GLN B 793      16.897  15.817 -51.694  1.00 61.88
ATOM   2937  CG  GLN B 793      17.928  15.613 -52.782  1.00 64.34
ATOM   2938  CD  GLN B 793      18.587  16.913 -53.200  1.00 65.85
ATOM   2939  OE1 GLN B 793      19.084  17.033 -54.317  1.00 67.77
ATOM   2940  NE2 GLN B 793      18.601  17.893 -52.299  1.00 66.10
ATOM   2941  N   LEU B 794      15.213  14.697 -49.072  1.00 58.48
ATOM   2942  CA  LEU B 794      14.250  15.036 -48.042  1.00 57.14
ATOM   2943  C   LEU B 794      14.689  16.346 -47.414  1.00 57.64
ATOM   2944  O   LEU B 794      15.859  16.531 -47.093  1.00 57.64
ATOM   2945  CB  LEU B 794      14.187  13.922 -46.992  1.00 55.84
ATOM   2946  CG  LEU B 794      13.804  12.529 -47.515  1.00 54.27
ATOM   2947  CD1 LEU B 794      13.456  11.624 -46.344  1.00 53.66
ATOM   2948  CD2 LEU B 794      12.616  12.627 -48.449  1.00 53.08
ATOM   2949  N   VAL B 795      13.746  17.264 -47.258  1.00 59.07
ATOM   2950  CA  VAL B 795      14.047  18.567 -46.690  1.00 59.85
ATOM   2951  C   VAL B 795      13.222  18.812 -45.435  1.00 62.17
ATOM   2952  O   VAL B 795      11.987  18.855 -45.472  1.00 61.88
ATOM   2953  CB  VAL B 795      13.774  19.697 -47.714  1.00 58.39
ATOM   2954  CG1 VAL B 795      14.231  21.040 -47.157  1.00 58.05
ATOM   2955  CG2 VAL B 795      14.495  19.394 -49.014  1.00 58.45
ATOM   2956  N   THR B 796      13.931  18.969 -44.323  1.00 63.79
ATOM   2957  CA  THR B 796      13.311  19.210 -43.034  1.00 65.36
```

```
ATOM   2958  C   THR B 796     13.869  20.476 -42.436  1.00 66.46
ATOM   2959  O   THR B 796     14.993  20.890 -42.747  1.00 66.26
ATOM   2960  CB  THR B 796     13.606  18.077 -42.033  1.00 65.06
ATOM   2961  OG1 THR B 796     13.043  16.852 -42.509  1.00 68.33
ATOM   2962  CG2 THR B 796     13.007  18.401 -40.672  1.00 66.50
ATOM   2963  N   GLN B 797     13.068  21.090 -41.574  1.00 66.67
ATOM   2964  CA  GLN B 797     13.488  22.284 -40.884  1.00 66.57
ATOM   2965  C   GLN B 797     14.690  21.827 -40.085  1.00 66.07
ATOM   2966  O   GLN B 797     14.680  20.741 -39.501  1.00 65.39
ATOM   2967  CB  GLN B 797     12.393  22.758 -39.935  1.00 67.57
ATOM   2968  CG  GLN B 797     12.673  24.081 -39.263  1.00 70.20
ATOM   2969  CD  GLN B 797     11.514  24.526 -38.399  1.00 73.88
ATOM   2970  OE1 GLN B 797     11.403  24.140 -37.230  1.00 75.03
ATOM   2971  NE2 GLN B 797     10.623  25.327 -38.979  1.00 74.39
ATOM   2972  N   LEU B 798     15.737  22.638 -40.083  1.00 66.31
ATOM   2973  CA  LEU B 798     16.931  22.303 -39.333  1.00 65.46
ATOM   2974  C   LEU B 798     16.672  22.549 -37.851  1.00 66.20
ATOM   2975  O   LEU B 798     15.902  23.441 -37.476  1.00 65.77
ATOM   2976  CB  LEU B 798     18.097  23.170 -39.791  1.00 64.87
ATOM   2977  CG  LEU B 798     19.410  22.965 -39.045  1.00 65.11
ATOM   2978  CD1 LEU B 798     19.933  21.554 -39.290  1.00 64.89
ATOM   2979  CD2 LEU B 798     20.411  23.999 -39.516  1.00 64.74
ATOM   2980  N   MET B 799     17.296  21.733 -37.011  1.00 66.39
ATOM   2981  CA  MET B 799     17.169  21.885 -35.571  1.00 65.45
ATOM   2982  C   MET B 799     18.506  22.465 -35.113  1.00 65.57
ATOM   2983  O   MET B 799     19.547  21.798 -35.162  1.00 64.60
ATOM   2984  CB  MET B 799     16.881  20.536 -34.911  1.00 64.87
ATOM   2985  CG  MET B 799     15.491  19.990 -35.216  1.00 64.16
ATOM   2986  SD  MET B 799     14.163  21.040 -34.582  1.00 65.40
ATOM   2987  CE  MET B 799     13.635  21.891 -36.058  1.00 64.20
ATOM   2988  N   PRO B 800     18.486  23.730 -34.669  1.00 65.90
ATOM   2989  CA  PRO B 800     19.652  24.484 -34.196  1.00 65.62
ATOM   2990  C   PRO B 800     20.591  23.765 -33.239  1.00 65.08
ATOM   2991  O   PRO B 800     21.805  23.817 -33.412  1.00 64.72
ATOM   2992  CB  PRO B 800     19.025  25.731 -33.566  1.00 66.58
ATOM   2993  CG  PRO B 800     17.699  25.239 -33.092  1.00 66.63
ATOM   2994  CD  PRO B 800     17.241  24.410 -34.269  1.00 66.65
ATOM   2995  N   HIS B 801     20.044  23.088 -32.237  1.00 63.99
ATOM   2996  CA  HIS B 801     20.892  22.408 -31.277  1.00 62.97
ATOM   2997  C   HIS B 801     21.310  20.988 -31.636  1.00 61.86
ATOM   2998  O   HIS B 801     21.843  20.257 -30.804  1.00 63.07
ATOM   2999  CB  HIS B 801     20.238  22.471 -29.900  1.00 64.77
ATOM   3000  CG  HIS B 801     20.298  23.836 -29.283  1.00 66.40
ATOM   3001  ND1 HIS B 801     21.486  24.432 -28.909  1.00 65.11
ATOM   3002  CD2 HIS B 801     19.324  24.740 -29.016  1.00 66.09
```

ATOM 3003 CE1 HIS B 801 21.240 25.641 -28.439 1.00 64.78
ATOM 3004 NE2 HIS B 801 19.936 25.853 -28.492 1.00 65.44
ATOM 3005 N GLY B 802 21.090 20.607 -32.886 1.00 60.15
ATOM 3006 CA GLY B 802 21.490 19.289 -33.331 1.00 57.51
ATOM 3007 C GLY B 802 20.901 18.064 -32.650 1.00 56.35
ATOM 3008 O GLY B 802 19.810 18.086 -32.075 1.00 53.17
ATOM 3009 N CYS B 803 21.660 16.978 -32.735 1.00 56.15
ATOM 3010 CA CYS B 803 21.277 15.688 -32.190 1.00 55.11
ATOM 3011 C CYS B 803 21.445 15.568 -30.682 1.00 55.33
ATOM 3012 O CYS B 803 22.491 15.911 -30.128 1.00 54.75
ATOM 3013 CB CYS B 803 22.074 14.594 -32.899 1.00 55.30
ATOM 3014 SG CYS B 803 21.743 14.518 -34.697 1.00 60.15
ATOM 3015 N LEU B 804 20.396 15.066 -30.031 1.00 54.33
ATOM 3016 CA LEU B 804 20.376 14.883 -28.588 1.00 53.12
ATOM 3017 C LEU B 804 21.534 14.014 -28.089 1.00 52.92
ATOM 3018 O LEU B 804 22.177 14.328 -27.088 1.00 51.69
ATOM 3019 CB LEU B 804 19.043 14.266 -28.168 1.00 52.44
ATOM 3020 CG LEU B 804 18.815 14.078 -26.666 1.00 50.62
ATOM 3021 CD1 LEU B 804 18.967 15.417 -25.974 1.00 51.38
ATOM 3022 CD2 LEU B 804 17.428 13.491 -26.413 1.00 49.29
ATOM 3023 N LEU B 805 21.801 12.920 -28.782 1.00 52.39
ATOM 3024 CA LEU B 805 22.888 12.053 -28.373 1.00 54.68
ATOM 3025 C LEU B 805 24.161 12.863 -28.138 1.00 57.25
ATOM 3026 O LEU B 805 24.918 12.604 -27.200 1.00 56.94
ATOM 3027 CB LEU B 805 23.156 10.998 -29.438 1.00 52.27
ATOM 3028 CG LEU B 805 24.380 10.169 -29.080 1.00 51.83
ATOM 3029 CD1 LEU B 805 24.151 9.471 -27.737 1.00 50.62
ATOM 3030 CD2 LEU B 805 24.660 9.179 -30.182 1.00 53.24
ATOM 3031 N GLU B 806 24.387 13.844 -29.006 1.00 60.22
ATOM 3032 CA GLU B 806 25.558 14.705 -28.919 1.00 62.56
ATOM 3033 C GLU B 806 25.351 15.761 -27.836 1.00 60.94
ATOM 3034 O GLU B 806 26.233 16.013 -27.018 1.00 60.73
ATOM 3035 CB GLU B 806 25.804 15.395 -30.267 1.00 67.71
ATOM 3036 CG GLU B 806 25.695 14.471 -31.488 1.00 75.24
ATOM 3037 CD GLU B 806 25.922 15.212 -32.804 1.00 79.21
ATOM 3038 OE1 GLU B 806 25.254 16.251 -33.026 1.00 81.47
ATOM 3039 OE2 GLU B 806 26.762 14.758 -33.615 1.00 79.92
ATOM 3040 N TYR B 807 24.173 16.371 -27.832 1.00 59.29
ATOM 3041 CA TYR B 807 23.856 17.400 -26.860 1.00 59.19
ATOM 3042 C TYR B 807 24.157 16.981 -25.424 1.00 59.38
ATOM 3043 O TYR B 807 24.822 17.708 -24.700 1.00 58.77
ATOM 3044 CB TYR B 807 22.391 17.784 -26.966 1.00 59.99
ATOM 3045 CG TYR B 807 22.053 19.071 -26.262 1.00 60.81
ATOM 3046 CD1 TYR B 807 22.227 20.300 -26.897 1.00 61.13
ATOM 3047 CD2 TYR B 807 21.546 19.064 -24.966 1.00 61.33

ATOM 3048 CE1 TYR B 807 21.899 21.489 -26.265 1.00 61.63
ATOM 3049 CE2 TYR B 807 21.215 20.252 -24.319 1.00 62.89
ATOM 3050 CZ TYR B 807 21.392 21.460 -24.977 1.00 62.83
ATOM 3051 OH TYR B 807 21.035 22.630 -24.354 1.00 64.52
ATOM 3052 N VAL B 808 23.671 15.819 -25.002 1.00 60.10
ATOM 3053 CA VAL B 808 23.927 15.382 -23.630 1.00 62.18
ATOM 3054 C VAL B 808 25.398 15.164 -23.325 1.00 63.86
ATOM 3055 O VAL B 808 25.855 15.480 -22.235 1.00 64.12
ATOM 3056 CB VAL B 808 23.176 14.073 -23.257 1.00 60.51
ATOM 3057 CG1 VAL B 808 21.704 14.344 -23.088 1.00 59.12
ATOM 3058 CG2 VAL B 808 23.417 13.015 -24.310 1.00 60.89
ATOM 3059 N HIS B 809 26.147 14.624 -24.273 1.00 67.06
ATOM 3060 CA HIS B 809 27.555 14.383 -24.014 1.00 70.40
ATOM 3061 C HIS B 809 28.269 15.679 -23.658 1.00 70.99
ATOM 3062 O HIS B 809 28.886 15.797 -22.602 1.00 72.12
ATOM 3063 CB HIS B 809 28.236 13.746 -25.226 1.00 73.29
ATOM 3064 CG HIS B 809 29.639 13.294 -24.956 1.00 76.84
ATOM 3065 ND1 HIS B 809 29.937 12.293 -24.056 1.00 77.14
ATOM 3066 CD2 HIS B 809 30.826 13.724 -25.447 1.00 77.99
ATOM 3067 CE1 HIS B 809 31.247 12.126 -24.005 1.00 78.08
ATOM 3068 NE2 HIS B 809 31.809 12.982 -24.839 1.00 78.17
ATOM 3069 N GLU B 810 28.162 16.660 -24.537 1.00 71.44
ATOM 3070 CA GLU B 810 28.827 17.928 -24.322 1.00 72.20
ATOM 3071 C GLU B 810 28.320 18.741 -23.141 1.00 72.35
ATOM 3072 O GLU B 810 29.121 19.284 -22.378 1.00 72.42
ATOM 3073 CB GLU B 810 28.760 18.741 -25.604 1.00 74.24
ATOM 3074 CG GLU B 810 29.503 18.067 -26.746 1.00 76.99
ATOM 3075 CD GLU B 810 29.191 18.694 -28.082 1.00 80.01
ATOM 3076 OE1 GLU B 810 29.408 19.918 -28.231 1.00 81.26
ATOM 3077 OE2 GLU B 810 28.726 17.961 -28.982 1.00 80.87
ATOM 3078 N HIS B 811 27.001 18.822 -22.976 1.00 72.11
ATOM 3079 CA HIS B 811 26.427 19.588 -21.869 1.00 71.84
ATOM 3080 C HIS B 811 26.168 18.752 -20.624 1.00 71.80
ATOM 3081 O HIS B 811 25.302 19.096 -19.820 1.00 70.61
ATOM 3082 CB HIS B 811 25.115 20.252 -22.286 1.00 71.49
ATOM 3083 CG HIS B 811 25.243 21.157 -23.468 1.00 71.98
ATOM 3084 ND1 HIS B 811 25.549 20.695 -24.729 1.00 73.94
ATOM 3085 CD2 HIS B 811 25.085 22.496 -23.586 1.00 72.36
ATOM 3086 CE1 HIS B 811 25.571 21.709 -25.575 1.00 74.46
ATOM 3087 NE2 HIS B 811 25.293 22.813 -24.907 1.00 74.62
ATOM 3088 N LYS B 812 26.917 17.665 -20.460 1.00 73.21
ATOM 3089 CA LYS B 812 26.736 16.793 -19.300 1.00 75.11
ATOM 3090 C LYS B 812 26.604 17.575 -18.001 1.00 75.97
ATOM 3091 O LYS B 812 25.592 17.499 -17.305 1.00 75.98
ATOM 3092 CB LYS B 812 27.901 15.805 -19.157 1.00 74.11

ATOM 3093 CG LYS B 812 27.887 15.118 -17.799 1.00 74.38
ATOM 3094 CD LYS B 812 28.809 13.917 -17.690 1.00 73.97
ATOM 3095 CE LYS B 812 28.613 13.265 -16.322 1.00 72.70
ATOM 3096 NZ LYS B 812 29.394 12.015 -16.154 1.00 73.35
ATOM 3097 N ASP B 813 27.642 18.330 -17.682 1.00 77.79
ATOM 3098 CA ASP B 813 27.668 19.119 -16.463 1.00 79.44
ATOM 3099 C ASP B 813 26.644 20.256 -16.500 1.00 79.12
ATOM 3100 O ASP B 813 26.706 21.185 -15.699 1.00 79.20
ATOM 3101 CB ASP B 813 29.085 19.659 -16.258 1.00 81.16
ATOM 3102 CG ASP B 813 30.154 18.594 -16.504 1.00 83.14
ATOM 3103 OD1 ASP B 813 30.044 17.498 -15.912 1.00 82.59
ATOM 3104 OD2 ASP B 813 31.101 18.845 -17.288 1.00 84.71
ATOM 3105 N ASN B 814 25.688 20.159 -17.421 1.00 78.87
ATOM 3106 CA ASN B 814 24.653 21.178 -17.570 1.00 77.92
ATOM 3107 C ASN B 814 23.247 20.591 -17.474 1.00 75.00
ATOM 3108 O ASN B 814 22.278 21.320 -17.278 1.00 73.54
ATOM 3109 CB ASN B 814 24.807 21.875 -18.925 1.00 83.27
ATOM 3110 CG ASN B 814 23.809 23.011 -19.123 1.00 87.37
ATOM 3111 OD1 ASN B 814 23.599 23.487 -20.248 1.00 89.03
ATOM 3112 ND2 ASN B 814 23.200 23.462 -18.027 1.00 88.12
ATOM 3113 N ILE B 815 23.136 19.274 -17.610 1.00 72.06
ATOM 3114 CA ILE B 815 21.834 18.608 -17.567 1.00 68.21
ATOM 3115 C ILE B 815 21.335 18.306 -16.157 1.00 65.98
ATOM 3116 O ILE B 815 22.010 17.630 -15.374 1.00 66.13
ATOM 3117 CB ILE B 815 21.864 17.285 -18.361 1.00 67.26
ATOM 3118 CG1 ILE B 815 22.485 17.517 -19.738 1.00 66.10
ATOM 3119 CG2 ILE B 815 20.461 16.739 -18.512 1.00 66.10
ATOM 3120 CD1 ILE B 815 21.770 18.532 -20.565 1.00 65.00
ATOM 3121 N GLY B 816 20.139 18.806 -15.853 1.00 63.12
ATOM 3122 CA GLY B 816 19.534 18.592 -14.549 1.00 59.27
ATOM 3123 C GLY B 816 18.502 17.479 -14.584 1.00 57.42
ATOM 3124 O GLY B 816 18.077 17.046 -15.658 1.00 56.24
ATOM 3125 N SER B 817 18.081 17.013 -13.413 1.00 53.84
ATOM 3126 CA SER B 817 17.118 15.936 -13.375 1.00 51.45
ATOM 3127 C SER B 817 15.826 16.343 -14.067 1.00 50.87
ATOM 3128 O SER B 817 15.205 15.532 -14.746 1.00 51.59
ATOM 3129 CB SER B 817 16.841 15.493 -11.927 1.00 50.35
ATOM 3130 OG SER B 817 16.050 16.422 -11.214 1.00 48.83
ATOM 3131 N GLN B 818 15.426 17.597 -13.914 1.00 48.39
ATOM 3132 CA GLN B 818 14.189 18.046 -14.531 1.00 50.14
ATOM 3133 C GLN B 818 14.256 17.872 -16.048 1.00 50.37
ATOM 3134 O GLN B 818 13.397 17.234 -16.664 1.00 50.57
ATOM 3135 CB GLN B 818 13.931 19.509 -14.172 1.00 51.39
ATOM 3136 CG GLN B 818 12.530 20.005 -14.512 1.00 53.65
ATOM 3137 CD GLN B 818 12.304 21.465 -14.104 1.00 54.44

ATOM 3138 OE1 GLN B 818 13.090 22.354 -14.451 1.00 51.78
ATOM 3139 NE2 GLN B 818 11.223 21.711 -13.374 1.00 53.12
ATOM 3140 N LEU B 819 15.299 18.439 -16.636 1.00 49.58
ATOM 3141 CA LEU B 819 15.542 18.376 -18.071 1.00 48.96
ATOM 3142 C LEU B 819 15.433 16.942 -18.617 1.00 48.91
ATOM 3143 O LEU B 819 14.665 16.680 -19.537 1.00 47.63
ATOM 3144 CB LEU B 819 16.937 18.931 -18.342 1.00 49.33
ATOM 3145 CG LEU B 819 17.233 19.667 -19.638 1.00 50.99
ATOM 3146 CD1 LEU B 819 16.180 20.729 -19.883 1.00 51.26
ATOM 3147 CD2 LEU B 819 18.620 20.284 -19.528 1.00 48.42
ATOM 3148 N LEU B 820 16.207 16.027 -18.036 1.00 48.12
ATOM 3149 CA LEU B 820 16.232 14.627 -18.448 1.00 47.03
ATOM 3150 C LEU B 820 14.908 13.879 -18.355 1.00 47.74
ATOM 3151 O LEU B 820 14.621 13.036 -19.210 1.00 46.11
ATOM 3152 CB LEU B 820 17.284 13.865 -17.648 1.00 46.94
ATOM 3153 CG LEU B 820 18.733 14.082 -18.069 1.00 46.17
ATOM 3154 CD1 LEU B 820 19.655 13.512 -17.010 1.00 48.56
ATOM 3155 CD2 LEU B 820 18.982 13.429 -19.417 1.00 47.04
ATOM 3156 N LEU B 821 14.119 14.159 -17.315 1.00 47.54
ATOM 3157 CA LEU B 821 12.818 13.508 -17.140 1.00 47.15
ATOM 3158 C LEU B 821 11.781 14.084 -18.094 1.00 47.22
ATOM 3159 O LEU B 821 10.822 13.407 -18.463 1.00 48.21
ATOM 3160 CB LEU B 821 12.311 13.667 -15.712 1.00 46.22
ATOM 3161 CG LEU B 821 12.974 12.829 -14.621 1.00 48.11
ATOM 3162 CD1 LEU B 821 12.444 13.272 -13.264 1.00 46.19
ATOM 3163 CD2 LEU B 821 12.685 11.353 -14.844 1.00 46.08
ATOM 3164 N ASN B 822 11.970 15.336 -18.489 1.00 47.10
ATOM 3165 CA ASN B 822 11.048 15.981 -19.415 1.00 48.36
ATOM 3166 C ASN B 822 11.311 15.539 -20.860 1.00 46.42
ATOM 3167 O ASN B 822 10.398 15.478 -21.678 1.00 46.12
ATOM 3168 CB ASN B 822 11.153 17.499 -19.263 1.00 52.20
ATOM 3169 CG ASN B 822 10.430 18.003 -18.020 1.00 56.94
ATOM 3170 OD1 ASN B 822 9.200 18.106 -18.005 1.00 60.36
ATOM 3171 ND2 ASN B 822 11.184 18.295 -16.966 1.00 58.16
ATOM 3172 N TRP B 823 12.560 15.220 -21.174 1.00 45.04
ATOM 3173 CA TRP B 823 12.878 14.746 -22.512 1.00 43.92
ATOM 3174 C TRP B 823 12.219 13.378 -22.647 1.00 43.43
ATOM 3175 O TRP B 823 11.667 13.026 -23.698 1.00 42.53
ATOM 3176 CB TRP B 823 14.390 14.597 -22.700 1.00 42.86
ATOM 3177 CG TRP B 823 15.149 15.901 -22.828 1.00 44.63
ATOM 3178 CD1 TRP B 823 14.654 17.109 -23.246 1.00 43.05
ATOM 3179 CD2 TRP B 823 16.553 16.098 -22.612 1.00 44.09
ATOM 3180 NE1 TRP B 823 15.664 18.036 -23.308 1.00 43.18
ATOM 3181 CE2 TRP B 823 16.840 17.445 -22.923 1.00 44.18
ATOM 3182 CE3 TRP B 823 17.599 15.264 -22.184 1.00 44.59

ATOM 3183 CZ2 TRP B 823 18.133 17.985 -22.818 1.00 44.47
ATOM 3184 CZ3 TRP B 823 18.886 15.803 -22.080 1.00 46.01
ATOM 3185 CH2 TRP B 823 19.139 17.154 -22.397 1.00 42.03
ATOM 3186 N CYS B 824 12.274 12.617 -21.560 1.00 41.79
ATOM 3187 CA CYS B 824 11.699 11.290 -21.535 1.00 42.66
ATOM 3188 C CYS B 824 10.243 11.359 -21.920 1.00 44.42
ATOM 3189 O CYS B 824 9.785 10.604 -22.778 1.00 45.73
ATOM 3190 CB CYS B 824 11.846 10.663 -20.144 1.00 43.86
ATOM 3191 SG CYS B 824 13.522 10.059 -19.758 1.00 43.47
ATOM 3192 N VAL B 825 9.521 12.278 -21.287 1.00 45.21
ATOM 3193 CA VAL B 825 8.100 12.455 -21.549 1.00 42.85
ATOM 3194 C VAL B 825 7.858 12.902 -22.979 1.00 42.45
ATOM 3195 O VAL B 825 6.970 12.394 -23.665 1.00 40.16
ATOM 3196 CB VAL B 825 7.486 13.495 -20.585 1.00 42.45
ATOM 3197 CG1 VAL B 825 6.062 13.834 -21.014 1.00 41.54
ATOM 3198 CG2 VAL B 825 7.488 12.948 -19.173 1.00 40.00
ATOM 3199 N GLN B 826 8.650 13.868 -23.423 1.00 43.25
ATOM 3200 CA GLN B 826 8.510 14.379 -24.776 1.00 43.45
ATOM 3201 C GLN B 826 8.769 13.251 -25.762 1.00 41.87
ATOM 3202 O GLN B 826 7.985 13.044 -26.685 1.00 42.00
ATOM 3203 CB GLN B 826 9.468 15.555 -25.000 1.00 42.33
ATOM 3204 CG GLN B 826 9.022 16.786 -24.250 1.00 44.18
ATOM 3205 CD GLN B 826 9.988 17.944 -24.348 1.00 44.47
ATOM 3206 OE1 GLN B 826 10.716 18.084 -25.321 1.00 43.53
ATOM 3207 NE2 GLN B 826 9.981 18.799 -23.335 1.00 47.99
ATOM 3208 N ILE B 827 9.845 12.498 -25.565 1.00 39.85
ATOM 3209 CA ILE B 827 10.093 11.406 -26.487 1.00 40.62
ATOM 3210 C ILE B 827 8.928 10.412 -26.458 1.00 41.30
ATOM 3211 O ILE B 827 8.459 9.988 -27.513 1.00 43.72
ATOM 3212 CB ILE B 827 11.402 10.662 -26.178 1.00 39.44
ATOM 3213 CG1 ILE B 827 12.578 11.636 -26.275 1.00 38.32
ATOM 3214 CG2 ILE B 827 11.583 9.500 -27.171 1.00 37.20
ATOM 3215 CD1 ILE B 827 13.934 11.012 -26.017 1.00 37.82
ATOM 3216 N ALA B 828 8.448 10.059 -25.266 1.00 38.63
ATOM 3217 CA ALA B 828 7.347 9.113 -25.146 1.00 40.14
ATOM 3218 C ALA B 828 6.043 9.649 -25.728 1.00 42.58
ATOM 3219 O ALA B 828 5.185 8.881 -26.177 1.00 43.82
ATOM 3220 CB ALA B 828 7.140 8.723 -23.692 1.00 40.67
ATOM 3221 N LYS B 829 5.873 10.963 -25.722 1.00 44.00
ATOM 3222 CA LYS B 829 4.647 11.525 -26.273 1.00 43.33
ATOM 3223 C LYS B 829 4.656 11.428 -27.795 1.00 43.62
ATOM 3224 O LYS B 829 3.640 11.094 -28.401 1.00 44.41
ATOM 3225 CB LYS B 829 4.461 12.971 -25.809 1.00 43.70
ATOM 3226 CG LYS B 829 3.810 13.088 -24.433 1.00 41.95
ATOM 3227 CD LYS B 829 3.641 14.542 -24.038 1.00 44.96

ATOM 3228 CE LYS B 829 2.871 14.679 -22.747 1.00 47.02
ATOM 3229 NZ LYS B 829 2.772 16.101 -22.347 1.00 49.90
ATOM 3230 N GLY B 830 5.803 11.704 -28.410 1.00 42.29
ATOM 3231 CA GLY B 830 5.897 11.603 -29.854 1.00 42.16
ATOM 3232 C GLY B 830 5.631 10.178 -30.327 1.00 42.55
ATOM 3233 O GLY B 830 4.952 9.958 -31.336 1.00 43.40
ATOM 3234 N MET B 831 6.178 9.202 -29.611 1.00 41.44
ATOM 3235 CA MET B 831 5.955 7.811 -29.972 1.00 43.60
ATOM 3236 C MET B 831 4.450 7.563 -29.842 1.00 43.46
ATOM 3237 O MET B 831 3.840 6.886 -30.670 1.00 42.80
ATOM 3238 CB MET B 831 6.748 6.867 -29.042 1.00 43.14
ATOM 3239 CG MET B 831 8.267 6.966 -29.199 1.00 42.68
ATOM 3240 SD MET B 831 8.809 6.840 -30.938 1.00 43.27
ATOM 3241 CE MET B 831 8.511 5.103 -31.247 1.00 44.19
ATOM 3242 N MET B 832 3.860 8.142 -28.802 1.00 42.18
ATOM 3243 CA MET B 832 2.433 8.006 -28.549 1.00 43.21
ATOM 3244 C MET B 832 1.641 8.454 -29.780 1.00 42.04
ATOM 3245 O MET B 832 0.683 7.793 -30.201 1.00 40.20
ATOM 3246 CB MET B 832 2.062 8.866 -27.347 1.00 46.91
ATOM 3247 CG MET B 832 0.984 8.297 -26.452 1.00 50.62
ATOM 3248 SD MET B 832 0.679 9.445 -25.093 1.00 58.47
ATOM 3249 CE MET B 832 1.936 8.941 -24.018 1.00 53.62
ATOM 3250 N TYR B 833 2.066 9.581 -30.349 1.00 40.89
ATOM 3251 CA TYR B 833 1.439 10.157 -31.523 1.00 39.85
ATOM 3252 C TYR B 833 1.616 9.253 -32.734 1.00 41.61
ATOM 3253 O TYR B 833 0.714 9.143 -33.572 1.00 39.17
ATOM 3254 CB TYR B 833 2.048 11.521 -31.824 1.00 39.98
ATOM 3255 CG TYR B 833 1.369 12.250 -32.970 1.00 42.77
ATOM 3256 CD1 TYR B 833 0.311 13.147 -32.737 1.00 41.95
ATOM 3257 CD2 TYR B 833 1.787 12.053 -34.290 1.00 38.99
ATOM 3258 CE1 TYR B 833 -0.301 13.832 -33.798 1.00 38.79
ATOM 3259 CE2 TYR B 833 1.184 12.724 -35.345 1.00 38.68
ATOM 3260 CZ TYR B 833 0.145 13.612 -35.097 1.00 40.21
ATOM 3261 OH TYR B 833 -0.433 14.279 -36.159 1.00 40.82
ATOM 3262 N LEU B 834 2.784 8.619 -32.829 1.00 42.19
ATOM 3263 CA LEU B 834 3.080 7.721 -33.944 1.00 43.73
ATOM 3264 C LEU B 834 2.265 6.423 -33.844 1.00 44.01
ATOM 3265 O LEU B 834 1.736 5.937 -34.845 1.00 42.17
ATOM 3266 CB LEU B 834 4.584 7.384 -33.989 1.00 45.03
ATOM 3267 CG LEU B 834 5.669 8.440 -34.301 1.00 47.70
ATOM 3268 CD1 LEU B 834 7.028 7.851 -33.978 1.00 46.80
ATOM 3269 CD2 LEU B 834 5.649 8.858 -35.759 1.00 44.71
ATOM 3270 N GLU B 835 2.166 5.866 -32.640 1.00 44.61
ATOM 3271 CA GLU B 835 1.428 4.624 -32.444 1.00 48.10
ATOM 3272 C GLU B 835 -0.053 4.827 -32.708 1.00 50.02

```
ATOM   3273  O   GLU B 835     -0.735   3.937 -33.215  1.00 48.65
ATOM   3274  CB  GLU B 835      1.622   4.089 -31.027  1.00 48.14
ATOM   3275  CG  GLU B 835      0.745   2.893 -30.733  1.00 51.80
ATOM   3276  CD  GLU B 835      0.921   2.380 -29.327  1.00 55.96
ATOM   3277  OE1 GLU B 835      1.020   3.212 -28.401  1.00 58.77
ATOM   3278  OE2 GLU B 835      0.949   1.147 -29.139  1.00 59.79
ATOM   3279  N   GLU B 836     -0.537   6.008 -32.347  1.00 51.95
ATOM   3280  CA  GLU B 836     -1.926   6.378 -32.545  1.00 53.09
ATOM   3281  C   GLU B 836     -2.227   6.270 -34.048  1.00 52.44
ATOM   3282  O   GLU B 836     -3.325   5.874 -34.442  1.00 52.73
ATOM   3283  CB  GLU B 836     -2.121   7.807 -32.029  1.00 55.57
ATOM   3284  CG  GLU B 836     -3.548   8.296 -31.901  1.00 62.73
ATOM   3285  CD  GLU B 836     -3.630   9.684 -31.243  1.00 69.86
ATOM   3286  OE1 GLU B 836     -4.721  10.308 -31.286  1.00 71.77
ATOM   3287  OE2 GLU B 836     -2.606  10.150 -30.677  1.00 71.84
ATOM   3288  N   ARG B 837     -1.233   6.597 -34.875  1.00 50.86
ATOM   3289  CA  ARG B 837     -1.361   6.550 -36.339  1.00 51.45
ATOM   3290  C   ARG B 837     -0.926   5.206 -36.939  1.00 50.30
ATOM   3291  O   ARG B 837     -0.750   5.098 -38.148  1.00 47.12
ATOM   3292  CB  ARG B 837     -0.501   7.650 -36.987  1.00 53.02
ATOM   3293  CG  ARG B 837     -0.781   9.066 -36.521  1.00 55.22
ATOM   3294  CD  ARG B 837     -2.239   9.377 -36.704  1.00 58.03
ATOM   3295  NE  ARG B 837     -2.603  10.765 -36.431  1.00 59.91
ATOM   3296  CZ  ARG B 837     -2.371  11.412 -35.294  1.00 58.31
ATOM   3297  NH1 ARG B 837     -1.745  10.822 -34.282  1.00 57.92
ATOM   3298  NH2 ARG B 837     -2.830  12.645 -35.152  1.00 57.89
ATOM   3299  N   ARG B 838     -0.754   4.198 -36.086  1.00 51.66
ATOM   3300  CA  ARG B 838     -0.295   2.864 -36.489  1.00 51.85
ATOM   3301  C   ARG B 838      1.055   2.920 -37.202  1.00 49.65
ATOM   3302  O   ARG B 838      1.290   2.213 -38.186  1.00 50.29
ATOM   3303  CB  ARG B 838     -1.334   2.143 -37.369  1.00 53.63
ATOM   3304  CG  ARG B 838     -2.470   1.492 -36.575  1.00 59.68
ATOM   3305  CD  ARG B 838     -1.932   0.532 -35.496  1.00 64.00
ATOM   3306  NE  ARG B 838     -1.885  -0.866 -35.933  1.00 69.82
ATOM   3307  CZ  ARG B 838     -2.913  -1.717 -35.876  1.00 71.87
ATOM   3308  NH1 ARG B 838     -2.764  -2.966 -36.307  1.00 71.46
ATOM   3309  NH2 ARG B 838     -4.084  -1.332 -35.374  1.00 72.32
ATOM   3310  N   LEU B 839      1.945   3.759 -36.692  1.00 45.08
ATOM   3311  CA  LEU B 839      3.263   3.886 -37.282  1.00 44.44
ATOM   3312  C   LEU B 839      4.350   3.426 -36.319  1.00 44.15
ATOM   3313  O   LEU B 839      4.454   3.900 -35.183  1.00 43.92
ATOM   3314  CB  LEU B 839      3.512   5.331 -37.699  1.00 45.11
ATOM   3315  CG  LEU B 839      2.429   5.939 -38.601  1.00 47.37
ATOM   3316  CD1 LEU B 839      2.763   7.407 -38.852  1.00 45.99
ATOM   3317  CD2 LEU B 839      2.317   5.161 -39.921  1.00 43.39
```

```
ATOM   3318  N   VAL B 840      5.152   2.481 -36.785  1.00 43.12
ATOM   3319  CA  VAL B 840      6.246   1.936 -36.000  1.00 42.97
ATOM   3320  C   VAL B 840      7.543   2.589 -36.490  1.00 43.65
ATOM   3321  O   VAL B 840      7.796   2.628 -37.690  1.00 44.79
ATOM   3322  CB  VAL B 840      6.305   0.408 -36.192  1.00 42.39
ATOM   3323  CG1 VAL B 840      7.382  -0.221 -35.307  1.00 42.09
ATOM   3324  CG2 VAL B 840      4.945  -0.177 -35.881  1.00 41.99
ATOM   3325  N   HIS B 841      8.351   3.110 -35.570  1.00 43.05
ATOM   3326  CA  HIS B 841      9.613   3.756 -35.932  1.00 43.35
ATOM   3327  C   HIS B 841     10.680   2.760 -36.412  1.00 44.72
ATOM   3328  O   HIS B 841     11.258   2.927 -37.485  1.00 45.10
ATOM   3329  CB  HIS B 841     10.150   4.547 -34.736  1.00 41.90
ATOM   3330  CG  HIS B 841     11.221   5.535 -35.090  1.00 40.88
ATOM   3331  ND1 HIS B 841     12.406   5.170 -35.690  1.00 39.11
ATOM   3332  CD2 HIS B 841     11.289   6.876 -34.917  1.00 41.53
ATOM   3333  CE1 HIS B 841     13.156   6.242 -35.870  1.00 40.04
ATOM   3334  NE2 HIS B 841     12.502   7.291 -35.409  1.00 39.97
ATOM   3335  N   ARG B 842     10.937   1.731 -35.607  1.00 46.60
ATOM   3336  CA  ARG B 842     11.927   0.691 -35.915  1.00 47.69
ATOM   3337  C   ARG B 842     13.380   1.106 -35.704  1.00 47.11
ATOM   3338  O   ARG B 842     14.260   0.250 -35.650  1.00 47.21
ATOM   3339  CB  ARG B 842     11.794   0.199 -37.356  1.00 48.94
ATOM   3340  CG  ARG B 842     10.483  -0.442 -37.701  1.00 53.39
ATOM   3341  CD  ARG B 842     10.558  -1.004 -39.106  1.00 56.65
ATOM   3342  NE  ARG B 842      9.354  -1.720 -39.505  1.00 57.96
ATOM   3343  CZ  ARG B 842      9.326  -2.590 -40.504  1.00 59.81
ATOM   3344  NH1 ARG B 842     10.435  -2.834 -41.183  1.00 61.66
ATOM   3345  NH2 ARG B 842      8.203  -3.216 -40.821  1.00 61.73
ATOM   3346  N   ASP B 843     13.639   2.403 -35.587  1.00 45.43
ATOM   3347  CA  ASP B 843     15.009   2.862 -35.402  1.00 44.93
ATOM   3348  C   ASP B 843     15.108   4.035 -34.427  1.00 43.50
ATOM   3349  O   ASP B 843     15.803   5.029 -34.679  1.00 40.29
ATOM   3350  CB  ASP B 843     15.602   3.234 -36.769  1.00 48.21
ATOM   3351  CG  ASP B 843     17.058   3.636 -36.687  1.00 49.17
ATOM   3352  OD1 ASP B 843     17.829   2.925 -36.005  1.00 50.67
ATOM   3353  OD2 ASP B 843     17.424   4.656 -37.309  1.00 50.03
ATOM   3354  N   LEU B 844     14.397   3.914 -33.312  1.00 41.09
ATOM   3355  CA  LEU B 844     14.409   4.942 -32.296  1.00 39.45
ATOM   3356  C   LEU B 844     15.683   4.757 -31.476  1.00 41.41
ATOM   3357  O   LEU B 844     15.962   3.662 -30.982  1.00 39.94
ATOM   3358  CB  LEU B 844     13.192   4.802 -31.394  1.00 37.57
ATOM   3359  CG  LEU B 844     13.136   5.718 -30.161  1.00 37.58
ATOM   3360  CD1 LEU B 844     12.897   7.175 -30.572  1.00 31.85
ATOM   3361  CD2 LEU B 844     12.023   5.232 -29.248  1.00 33.61
ATOM   3362  N   ALA B 845     16.461   5.825 -31.356  1.00 41.14
```

```
ATOM   3363  CA  ALA B 845      17.703   5.793 -30.594  1.00 43.80
ATOM   3364  C   ALA B 845      17.998   7.233 -30.239  1.00 44.77
ATOM   3365  O   ALA B 845      17.463   8.139 -30.872  1.00 46.46
ATOM   3366  CB  ALA B 845      18.839   5.208 -31.436  1.00 43.20
ATOM   3367  N   ALA B 846      18.838   7.462 -29.241  1.00 44.58
ATOM   3368  CA  ALA B 846      19.124   8.833 -28.856  1.00 45.24
ATOM   3369  C   ALA B 846      19.609   9.661 -30.030  1.00 45.63
ATOM   3370  O   ALA B 846      19.289  10.850 -30.115  1.00 47.93
ATOM   3371  CB  ALA B 846      20.142   8.870 -27.734  1.00 45.17
ATOM   3372  N   ARG B 847      20.363   9.045 -30.941  1.00 44.22
ATOM   3373  CA  ARG B 847      20.886   9.786 -32.094  1.00 46.27
ATOM   3374  C   ARG B 847      19.800  10.270 -33.054  1.00 46.18
ATOM   3375  O   ARG B 847      20.043  11.161 -33.865  1.00 46.55
ATOM   3376  CB  ARG B 847      21.895   8.951 -32.877  1.00 46.11
ATOM   3377  CG  ARG B 847      21.254   7.928 -33.760  1.00 49.88
ATOM   3378  CD  ARG B 847      22.263   7.195 -34.602  1.00 50.73
ATOM   3379  NE  ARG B 847      21.564   6.353 -35.565  1.00 57.37
ATOM   3380  CZ  ARG B 847      20.873   5.264 -35.242  1.00 58.79
ATOM   3381  NH1 ARG B 847      20.794   4.872 -33.976  1.00 60.01
ATOM   3382  NH2 ARG B 847      20.243   4.576 -36.182  1.00 59.64
ATOM   3383  N   ASN B 848      18.610   9.683 -32.978  1.00 45.11
ATOM   3384  CA  ASN B 848      17.532  10.114 -33.848  1.00 45.22
ATOM   3385  C   ASN B 848      16.525  11.015 -33.132  1.00 47.16
ATOM   3386  O   ASN B 848      15.351  11.117 -33.525  1.00 46.11
ATOM   3387  CB  ASN B 848      16.840   8.917 -34.500  1.00 43.37
ATOM   3388  CG  ASN B 848      17.576   8.434 -35.736  1.00 44.82
ATOM   3389  OD1 ASN B 848      17.953   9.234 -36.596  1.00 47.01
ATOM   3390  ND2 ASN B 848      17.781   7.127 -35.838  1.00 42.89
ATOM   3391  N   VAL B 849      16.996  11.657 -32.065  1.00 47.02
ATOM   3392  CA  VAL B 849      16.181  12.606 -31.330  1.00 48.04
ATOM   3393  C   VAL B 849      16.951  13.914 -31.472  1.00 48.97
ATOM   3394  O   VAL B 849      18.134  13.987 -31.146  1.00 49.90
ATOM   3395  CB  VAL B 849      16.026  12.235 -29.829  1.00 48.21
ATOM   3396  CG1 VAL B 849      15.223  13.322 -29.109  1.00 48.81
ATOM   3397  CG2 VAL B 849      15.298  10.899 -29.689  1.00 46.65
ATOM   3398  N   LEU B 850      16.281  14.934 -31.995  1.00 50.30
ATOM   3399  CA  LEU B 850      16.900  16.234 -32.216  1.00 49.70
ATOM   3400  C   LEU B 850      16.503  17.241 -31.144  1.00 51.97
ATOM   3401  O   LEU B 850      15.449  17.116 -30.514  1.00 53.21
ATOM   3402  CB  LEU B 850      16.490  16.768 -33.583  1.00 46.49
ATOM   3403  CG  LEU B 850      16.660  15.825 -34.771  1.00 45.29
ATOM   3404  CD1 LEU B 850      16.076  16.481 -35.999  1.00 43.36
ATOM   3405  CD2 LEU B 850      18.120  15.500 -34.986  1.00 44.40
ATOM   3406  N   VAL B 851      17.352  18.249 -30.954  1.00 53.33
ATOM   3407  CA  VAL B 851      17.112  19.284 -29.960  1.00 53.66
```

```
ATOM   3408  C   VAL B 851      16.731  20.610 -30.628  1.00 55.93
ATOM   3409  O   VAL B 851      17.595  21.317 -31.153  1.00 56.57
ATOM   3410  CB  VAL B 851      18.375  19.494 -29.094  1.00 52.04
ATOM   3411  CG1 VAL B 851      18.081  20.455 -27.966  1.00 53.25
ATOM   3412  CG2 VAL B 851      18.850  18.171 -28.540  1.00 50.16
ATOM   3413  N   LYS B 852      15.440  20.940 -30.624  1.00 57.66
ATOM   3414  CA  LYS B 852      14.982  22.196 -31.222  1.00 60.00
ATOM   3415  C   LYS B 852      15.497  23.295 -30.317  1.00 62.13
ATOM   3416  O   LYS B 852      15.977  24.328 -30.778  1.00 64.39
ATOM   3417  CB  LYS B 852      13.458  22.268 -31.272  1.00 58.87
ATOM   3418  CG  LYS B 852      12.923  23.615 -31.741  1.00 58.96
ATOM   3419  CD  LYS B 852      11.398  23.646 -31.691  1.00 60.41
ATOM   3420  CE  LYS B 852      10.817  24.892 -32.352  1.00 60.45
ATOM   3421  NZ  LYS B 852       9.312  24.862 -32.407  1.00 61.83
ATOM   3422  N   SER B 853      15.374  23.050 -29.017  1.00 61.87
ATOM   3423  CA  SER B 853      15.837  23.960 -27.980  1.00 61.38
ATOM   3424  C   SER B 853      15.945  23.145 -26.680  1.00 61.16
ATOM   3425  O   SER B 853      15.236  22.157 -26.489  1.00 58.97
ATOM   3426  CB  SER B 853      14.878  25.147 -27.822  1.00 59.92
ATOM   3427  OG  SER B 853      13.582  24.731 -27.445  1.00 61.79
ATOM   3428  N   PRO B 854      16.851  23.546 -25.780  1.00 61.17
ATOM   3429  CA  PRO B 854      17.076  22.865 -24.503  1.00 60.56
ATOM   3430  C   PRO B 854      15.876  22.143 -23.892  1.00 59.89
ATOM   3431  O   PRO B 854      15.957  20.959 -23.555  1.00 59.58
ATOM   3432  CB  PRO B 854      17.599  23.986 -23.625  1.00 61.16
ATOM   3433  CG  PRO B 854      18.478  24.738 -24.599  1.00 62.45
ATOM   3434  CD  PRO B 854      17.600  24.818 -25.834  1.00 62.08
ATOM   3435  N   ALA B 855      14.764  22.850 -23.762  1.00 57.36
ATOM   3436  CA  ALA B 855      13.576  22.269 -23.173  1.00 55.01
ATOM   3437  C   ALA B 855      12.621  21.699 -24.210  1.00 55.18
ATOM   3438  O   ALA B 855      11.440  21.533 -23.929  1.00 54.40
ATOM   3439  CB  ALA B 855      12.867  23.323 -22.354  1.00 54.10
ATOM   3440  N   HIS B 856      13.116  21.368 -25.399  1.00 55.23
ATOM   3441  CA  HIS B 856      12.222  20.881 -26.448  1.00 52.68
ATOM   3442  C   HIS B 856      12.891  19.970 -27.478  1.00 51.26
ATOM   3443  O   HIS B 856      13.649  20.427 -28.343  1.00 51.11
ATOM   3444  CB  HIS B 856      11.602  22.096 -27.148  1.00 53.04
ATOM   3445  CG  HIS B 856      10.492  21.766 -28.097  1.00 55.71
ATOM   3446  ND1 HIS B 856       9.868  22.714 -28.880  1.00 55.62
ATOM   3447  CD2 HIS B 856       9.902  20.583 -28.396  1.00 54.97
ATOM   3448  CE1 HIS B 856       8.943  22.129 -29.619  1.00 55.10
ATOM   3449  NE2 HIS B 856       8.942  20.837 -29.344  1.00 55.98
ATOM   3450  N   VAL B 857      12.602  18.677 -27.388  1.00 48.98
ATOM   3451  CA  VAL B 857      13.164  17.717 -28.328  1.00 47.33
ATOM   3452  C   VAL B 857      12.076  17.225 -29.291  1.00 46.32
```

ATOM 3453 O VAL B 857 10.877 17.362 -29.018 1.00 45.36
ATOM 3454 CB VAL B 857 13.827 16.500 -27.593 1.00 46.33
ATOM 3455 CG1 VAL B 857 15.094 16.944 -26.897 1.00 44.86
ATOM 3456 CG2 VAL B 857 12.874 15.902 -26.581 1.00 44.39
ATOM 3457 N LYS B 858 12.516 16.681 -30.425 1.00 44.31
ATOM 3458 CA LYS B 858 11.636 16.145 -31.459 1.00 43.59
ATOM 3459 C LYS B 858 12.222 14.849 -32.014 1.00 43.20
ATOM 3460 O LYS B 858 13.438 14.753 -32.217 1.00 43.70
ATOM 3461 CB LYS B 858 11.492 17.140 -32.614 1.00 44.67
ATOM 3462 CG LYS B 858 10.538 18.301 -32.362 1.00 46.35
ATOM 3463 CD LYS B 858 10.463 19.170 -33.610 1.00 46.33
ATOM 3464 CE LYS B 858 9.382 20.215 -33.508 1.00 46.98
ATOM 3465 NZ LYS B 858 9.214 20.892 -34.816 1.00 50.99
ATOM 3466 N ILE B 859 11.367 13.855 -32.265 1.00 42.00
ATOM 3467 CA ILE B 859 11.832 12.583 -32.816 1.00 39.14
ATOM 3468 C ILE B 859 11.955 12.719 -34.328 1.00 39.96
ATOM 3469 O ILE B 859 11.140 13.386 -34.966 1.00 40.22
ATOM 3470 CB ILE B 859 10.863 11.431 -32.480 1.00 37.12
ATOM 3471 CG1 ILE B 859 10.738 11.297 -30.958 1.00 37.67
ATOM 3472 CG2 ILE B 859 11.384 10.129 -33.069 1.00 34.33
ATOM 3473 CD1 ILE B 859 9.834 10.171 -30.480 1.00 33.72
ATOM 3474 N THR B 860 12.977 12.093 -34.900 1.00 41.18
ATOM 3475 CA THR B 860 13.197 12.174 -36.342 1.00 43.70
ATOM 3476 C THR B 860 13.596 10.844 -36.971 1.00 45.83
ATOM 3477 O THR B 860 14.019 9.918 -36.278 1.00 47.50
ATOM 3478 CB THR B 860 14.312 13.218 -36.688 1.00 42.70
ATOM 3479 OG1 THR B 860 14.311 13.486 -38.096 1.00 41.02
ATOM 3480 CG2 THR B 860 15.685 12.683 -36.317 1.00 41.73
ATOM 3481 N ASP B 861 13.463 10.772 -38.294 1.00 46.92
ATOM 3482 CA ASP B 861 13.839 9.597 -39.078 1.00 49.85
ATOM 3483 C ASP B 861 12.873 8.419 -39.058 1.00 50.50
ATOM 3484 O ASP B 861 13.233 7.317 -39.458 1.00 50.83
ATOM 3485 CB ASP B 861 15.239 9.109 -38.680 1.00 50.52
ATOM 3486 CG ASP B 861 16.070 8.688 -39.883 1.00 54.77
ATOM 3487 OD1 ASP B 861 16.304 9.533 -40.764 1.00 56.69
ATOM 3488 OD2 ASP B 861 16.495 7.518 -39.959 1.00 58.38
ATOM 3489 N PHE B 862 11.649 8.633 -38.600 1.00 52.16
ATOM 3490 CA PHE B 862 10.689 7.542 -38.606 1.00 55.68
ATOM 3491 C PHE B 862 10.256 7.323 -40.057 1.00 58.32
ATOM 3492 O PHE B 862 10.120 8.281 -40.823 1.00 59.56
ATOM 3493 CB PHE B 862 9.472 7.873 -37.732 1.00 55.12
ATOM 3494 CG PHE B 862 8.874 9.233 -37.995 1.00 54.59
ATOM 3495 CD1 PHE B 862 9.153 10.303 -37.149 1.00 54.37
ATOM 3496 CD2 PHE B 862 8.038 9.445 -39.085 1.00 53.46
ATOM 3497 CE1 PHE B 862 8.610 11.560 -37.385 1.00 53.72

ATOM 3498 CE2 PHE B 862 7.489 10.700 -39.331 1.00 52.07
ATOM 3499 CZ PHE B 862 7.777 11.757 -38.478 1.00 53.20
ATOM 3500 N GLY B 863 10.066 6.068 -40.446 1.00 60.33
ATOM 3501 CA GLY B 863 9.646 5.797 -41.809 1.00 64.81
ATOM 3502 C GLY B 863 10.679 5.163 -42.725 1.00 68.14
ATOM 3503 O GLY B 863 10.377 4.174 -43.393 1.00 68.10
ATOM 3504 N LEU B 864 11.887 5.726 -42.768 1.00 70.85
ATOM 3505 CA LEU B 864 12.952 5.194 -43.622 1.00 73.25
ATOM 3506 C LEU B 864 13.219 3.714 -43.386 1.00 74.47
ATOM 3507 O LEU B 864 13.373 2.950 -44.335 1.00 76.25
ATOM 3508 CB LEU B 864 14.267 5.949 -43.412 1.00 73.37
ATOM 3509 CG LEU B 864 14.399 7.414 -43.815 1.00 72.75
ATOM 3510 CD1 LEU B 864 15.853 7.800 -43.685 1.00 72.55
ATOM 3511 CD2 LEU B 864 13.925 7.633 -45.237 1.00 72.97
ATOM 3512 N ALA B 865 13.291 3.319 -42.121 1.00 74.99
ATOM 3513 CA ALA B 865 13.549 1.932 -41.769 1.00 75.61
ATOM 3514 C ALA B 865 12.791 0.967 -42.679 1.00 76.21
ATOM 3515 O ALA B 865 13.392 0.215 -43.456 1.00 76.63
ATOM 3516 CB ALA B 865 13.163 1.692 -40.322 1.00 76.18
ATOM 3517 N ARG B 866 11.467 1.001 -42.582 1.00 75.63
ATOM 3518 CA ARG B 866 10.615 0.127 -43.377 1.00 74.69
ATOM 3519 C ARG B 866 10.806 0.377 -44.866 1.00 72.85
ATOM 3520 O ARG B 866 10.788 -0.555 -45.672 1.00 72.17
ATOM 3521 CB ARG B 866 9.150 0.355 -43.010 1.00 77.16
ATOM 3522 CG ARG B 866 8.192 -0.678 -43.579 1.00 80.89
ATOM 3523 CD ARG B 866 6.766 -0.351 -43.162 1.00 84.67
ATOM 3524 NE ARG B 866 5.889 -1.518 -43.176 1.00 87.14
ATOM 3525 CZ ARG B 866 4.665 -1.535 -42.656 1.00 89.52
ATOM 3526 NH1 ARG B 866 4.169 -0.441 -42.081 1.00 89.56
ATOM 3527 NH2 ARG B 866 3.942 -2.648 -42.698 1.00 90.37
ATOM 3528 N LEU B 867 10.999 1.639 -45.229 1.00 69.43
ATOM 3529 CA LEU B 867 11.173 1.993 -46.630 1.00 68.73
ATOM 3530 C LEU B 867 12.416 1.394 -47.275 1.00 68.30
ATOM 3531 O LEU B 867 12.376 0.980 -48.433 1.00 68.60
ATOM 3532 CB LEU B 867 11.206 3.513 -46.801 1.00 67.15
ATOM 3533 CG LEU B 867 11.287 3.964 -48.258 1.00 63.74
ATOM 3534 CD1 LEU B 867 10.063 3.458 -49.008 1.00 62.81
ATOM 3535 CD2 LEU B 867 11.384 5.474 -48.331 1.00 61.46
ATOM 3536 N LEU B 868 13.516 1.348 -46.532 1.00 67.70
ATOM 3537 CA LEU B 868 14.759 0.810 -47.066 1.00 67.56
ATOM 3538 C LEU B 868 14.851 -0.703 -46.951 1.00 66.73
ATOM 3539 O LEU B 868 15.386 -1.361 -47.841 1.00 65.40
ATOM 3540 CB LEU B 868 15.963 1.446 -46.365 1.00 69.33
ATOM 3541 CG LEU B 868 15.984 2.976 -46.258 1.00 71.54
ATOM 3542 CD1 LEU B 868 17.337 3.418 -45.705 1.00 71.31

ATOM 3543 CD2 LEU B 868 15.719 3.613 -47.617 1.00 70.98
ATOM 3544 N GLU B 869 14.329 -1.263 -45.865 1.00 66.47
ATOM 3545 CA GLU B 869 14.393 -2.705 -45.692 1.00 66.24
ATOM 3546 C GLU B 869 13.191 -3.433 -46.271 1.00 65.56
ATOM 3547 O GLU B 869 13.276 -4.020 -47.345 1.00 66.35
ATOM 3548 CB GLU B 869 14.547 -3.055 -44.220 1.00 67.33
ATOM 3549 CG GLU B 869 15.784 -2.462 -43.592 1.00 69.61
ATOM 3550 CD GLU B 869 16.423 -3.390 -42.579 1.00 71.71
ATOM 3551 OE1 GLU B 869 15.728 -3.811 -41.620 1.00 70.66
ATOM 3552 OE2 GLU B 869 17.625 -3.697 -42.752 1.00 72.27
ATOM 3553 N GLY B 870 12.073 -3.396 -45.563 1.00 64.97
ATOM 3554 CA GLY B 870 10.888 -4.076 -46.041 1.00 64.73
ATOM 3555 C GLY B 870 10.238 -4.819 -44.900 1.00 65.26
ATOM 3556 O GLY B 870 10.555 -4.567 -43.744 1.00 64.41
ATOM 3557 N ASP B 871 9.344 -5.748 -45.216 1.00 66.68
ATOM 3558 CA ASP B 871 8.647 -6.501 -44.182 1.00 67.47
ATOM 3559 C ASP B 871 8.975 -7.982 -44.162 1.00 66.00
ATOM 3560 O ASP B 871 8.345 -8.747 -43.434 1.00 65.97
ATOM 3561 CB ASP B 871 7.137 -6.327 -44.351 1.00 72.20
ATOM 3562 CG ASP B 871 6.676 -4.927 -44.013 1.00 76.99
ATOM 3563 OD1 ASP B 871 6.783 -4.551 -42.824 1.00 80.07
ATOM 3564 OD2 ASP B 871 6.216 -4.204 -44.930 1.00 78.50
ATOM 3565 N GLU B 872 9.961 -8.389 -44.951 1.00 64.83
ATOM 3566 CA GLU B 872 10.333 -9.794 -45.018 1.00 63.94
ATOM 3567 C GLU B 872 10.666 -10.338 -43.631 1.00 61.57
ATOM 3568 O GLU B 872 11.580 -9.857 -42.963 1.00 60.56
ATOM 3569 CB GLU B 872 11.522 -9.969 -45.961 1.00 66.69
ATOM 3570 CG GLU B 872 11.932 -11.418 -46.172 1.00 71.91
ATOM 3571 CD GLU B 872 13.047 -11.569 -47.202 1.00 76.05
ATOM 3572 OE1 GLU B 872 13.408 -10.553 -47.842 1.00 76.98
ATOM 3573 OE2 GLU B 872 13.557 -12.702 -47.378 1.00 77.59
ATOM 3574 N ALA B 873 9.914 -11.342 -43.202 1.00 59.27
ATOM 3575 CA ALA B 873 10.124 -11.935 -41.894 1.00 57.77
ATOM 3576 C ALA B 873 11.549 -12.447 -41.719 1.00 58.33
ATOM 3577 O ALA B 873 12.171 -12.267 -40.668 1.00 56.59
ATOM 3578 CB ALA B 873 9.133 -13.070 -41.679 1.00 55.37
ATOM 3579 N ALA B 874 12.076 -13.086 -42.755 1.00 59.61
ATOM 3580 CA ALA B 874 13.418 -13.640 -42.666 1.00 60.12
ATOM 3581 C ALA B 874 14.500 -12.681 -43.134 1.00 60.09
ATOM 3582 O ALA B 874 14.395 -12.075 -44.203 1.00 60.48
ATOM 3583 CB ALA B 874 13.494 -14.949 -43.456 1.00 59.26
ATOM 3584 N TYR B 875 15.538 -12.542 -42.316 1.00 59.00
ATOM 3585 CA TYR B 875 16.667 -11.688 -42.655 1.00 58.29
ATOM 3586 C TYR B 875 17.575 -12.464 -43.595 1.00 58.10
ATOM 3587 O TYR B 875 17.824 -13.649 -43.388 1.00 57.86

```
ATOM   3588  CB  TYR B 875      17.487 -11.336 -41.414  1.00 58.23
ATOM   3589  CG  TYR B 875      16.842 -10.360 -40.466  1.00 58.80
ATOM   3590  CD1 TYR B 875      16.632  -9.033 -40.842  1.00 57.46
ATOM   3591  CD2 TYR B 875      16.456 -10.759 -39.185  1.00 56.30
ATOM   3592  CE1 TYR B 875      16.056  -8.126 -39.970  1.00 58.87
ATOM   3593  CE2 TYR B 875      15.879  -9.862 -38.303  1.00 59.49
ATOM   3594  CZ  TYR B 875      15.680  -8.543 -38.701  1.00 60.51
ATOM   3595  OH  TYR B 875      15.102  -7.645 -37.834  1.00 60.20
ATOM   3596  N   ASN B 876      18.060 -11.802 -44.634  1.00 58.32
ATOM   3597  CA  ASN B 876      18.984 -12.440 -45.550  1.00 58.92
ATOM   3598  C   ASN B 876      20.368 -12.237 -44.912  1.00 59.09
ATOM   3599  O   ASN B 876      20.457 -11.766 -43.775  1.00 57.47
ATOM   3600  CB  ASN B 876      18.879 -11.805 -46.943  1.00 59.97
ATOM   3601  CG  ASN B 876      18.810 -10.286 -46.903  1.00 65.32
ATOM   3602  OD1 ASN B 876      18.123  -9.696 -46.055  1.00 69.32
ATOM   3603  ND2 ASN B 876      19.505  -9.638 -47.836  1.00 65.71
ATOM   3604  N   ALA B 877      21.435 -12.596 -45.617  1.00 59.32
ATOM   3605  CA  ALA B 877      22.787 -12.466 -45.077  1.00 59.77
ATOM   3606  C   ALA B 877      23.238 -11.011 -44.883  1.00 61.45
ATOM   3607  O   ALA B 877      24.270 -10.746 -44.245  1.00 59.71
ATOM   3608  CB  ALA B 877      23.765 -13.201 -45.983  1.00 60.47
ATOM   3609  N   ASP B 878      22.459 -10.079 -45.434  1.00 62.48
ATOM   3610  CA  ASP B 878      22.753  -8.654 -45.334  1.00 62.92
ATOM   3611  C   ASP B 878      22.260  -8.132 -43.987  1.00 63.34
ATOM   3612  O   ASP B 878      22.660  -7.055 -43.548  1.00 63.62
ATOM   3613  CB  ASP B 878      22.067  -7.894 -46.479  1.00 62.83
ATOM   3614  CG  ASP B 878      22.688  -6.519 -46.737  1.00 64.73
ATOM   3615  OD1 ASP B 878      23.921  -6.442 -46.947  1.00 63.55
ATOM   3616  OD2 ASP B 878      21.938  -5.516 -46.745  1.00 64.59
ATOM   3617  N   GLY B 879      21.386  -8.902 -43.340  1.00 63.87
ATOM   3618  CA  GLY B 879      20.847  -8.516 -42.042  1.00 65.56
ATOM   3619  C   GLY B 879      19.955  -7.281 -42.027  1.00 65.90
ATOM   3620  O   GLY B 879      19.336  -6.933 -43.037  1.00 66.17
ATOM   3621  N   GLY B 880      19.885  -6.621 -40.873  1.00 65.12
ATOM   3622  CA  GLY B 880      19.074  -5.422 -40.754  1.00 64.82
ATOM   3623  C   GLY B 880      19.899  -4.157 -40.938  1.00 64.56
ATOM   3624  O   GLY B 880      21.107  -4.229 -41.141  1.00 64.99
ATOM   3625  N   ALA B 881      19.259  -2.995 -40.871  1.00 63.83
ATOM   3626  CA  ALA B 881      19.978  -1.736 -41.025  1.00 63.13
ATOM   3627  C   ALA B 881      20.131  -1.016 -39.686  1.00 62.11
ATOM   3628  O   ALA B 881      21.023  -0.188 -39.522  1.00 61.84
ATOM   3629  CB  ALA B 881      19.261  -0.835 -42.033  1.00 63.27
ATOM   3630  N   MET B 882      19.270  -1.334 -38.726  1.00 60.73
ATOM   3631  CA  MET B 882      19.346  -0.692 -37.422  1.00 60.66
ATOM   3632  C   MET B 882      20.388  -1.349 -36.543  1.00 57.66
```

ATOM 3633 O MET B 882 20.738 -2.505 -36.742 1.00 58.53
ATOM 3634 CB MET B 882 18.006 -0.759 -36.692 1.00 64.90
ATOM 3635 CG MET B 882 16.844 -0.168 -37.442 1.00 71.12
ATOM 3636 SD MET B 882 16.275 -1.292 -38.702 1.00 79.62
ATOM 3637 CE MET B 882 16.473 -0.256 -40.127 1.00 78.23
ATOM 3638 N PRO B 883 20.906 -0.610 -35.558 1.00 54.95
ATOM 3639 CA PRO B 883 21.910 -1.186 -34.666 1.00 54.93
ATOM 3640 C PRO B 883 21.262 -2.267 -33.804 1.00 54.49
ATOM 3641 O PRO B 883 20.201 -2.054 -33.239 1.00 55.33
ATOM 3642 CB PRO B 883 22.392 0.022 -33.869 1.00 54.23
ATOM 3643 CG PRO B 883 21.206 0.944 -33.882 1.00 55.31
ATOM 3644 CD PRO B 883 20.719 0.826 -35.291 1.00 53.61
ATOM 3645 N ILE B 884 21.904 -3.427 -33.710 1.00 55.18
ATOM 3646 CA ILE B 884 21.363 -4.549 -32.949 1.00 54.75
ATOM 3647 C ILE B 884 21.109 -4.230 -31.481 1.00 53.77
ATOM 3648 O ILE B 884 20.193 -4.778 -30.871 1.00 52.49
ATOM 3649 CB ILE B 884 22.315 -5.786 -32.997 1.00 57.45
ATOM 3650 CG1 ILE B 884 22.977 -5.911 -34.379 1.00 60.74
ATOM 3651 CG2 ILE B 884 21.522 -7.070 -32.704 1.00 56.49
ATOM 3652 CD1 ILE B 884 22.026 -6.282 -35.528 1.00 61.29
ATOM 3653 N LYS B 885 21.912 -3.333 -30.919 1.00 53.13
ATOM 3654 CA LYS B 885 21.809 -3.004 -29.499 1.00 51.92
ATOM 3655 C LYS B 885 20.604 -2.183 -29.040 1.00 50.73
ATOM 3656 O LYS B 885 20.309 -2.099 -27.850 1.00 50.67
ATOM 3657 CB LYS B 885 23.118 -2.350 -29.052 1.00 51.96
ATOM 3658 CG LYS B 885 24.316 -3.277 -29.214 1.00 49.00
ATOM 3659 CD LYS B 885 25.597 -2.616 -28.766 1.00 52.24
ATOM 3660 CE LYS B 885 26.798 -3.482 -29.122 1.00 53.83
ATOM 3661 NZ LYS B 885 28.091 -2.784 -28.862 1.00 56.01
ATOM 3662 N TRP B 886 19.900 -1.588 -29.985 1.00 48.96
ATOM 3663 CA TRP B 886 18.728 -0.797 -29.667 1.00 47.71
ATOM 3664 C TRP B 886 17.494 -1.600 -30.055 1.00 48.21
ATOM 3665 O TRP B 886 16.363 -1.142 -29.899 1.00 49.83
ATOM 3666 CB TRP B 886 18.765 0.501 -30.470 1.00 46.30
ATOM 3667 CG TRP B 886 19.594 1.587 -29.863 1.00 46.96
ATOM 3668 CD1 TRP B 886 19.138 2.657 -29.145 1.00 45.46
ATOM 3669 CD2 TRP B 886 21.014 1.750 -29.965 1.00 47.38
ATOM 3670 NE1 TRP B 886 20.182 3.480 -28.802 1.00 45.52
ATOM 3671 CE2 TRP B 886 21.346 2.950 -29.293 1.00 46.37
ATOM 3672 CE3 TRP B 886 22.039 1.003 -30.560 1.00 48.54
ATOM 3673 CZ2 TRP B 886 22.661 3.422 -29.202 1.00 44.45
ATOM 3674 CZ3 TRP B 886 23.354 1.479 -30.468 1.00 48.55
ATOM 3675 CH2 TRP B 886 23.648 2.678 -29.793 1.00 43.97
ATOM 3676 N MET B 887 17.731 -2.814 -30.536 1.00 47.39
ATOM 3677 CA MET B 887 16.689 -3.702 -31.038 1.00 47.29

```
ATOM   3678  C   MET B 887      16.042  -4.632 -30.021  1.00 46.15
ATOM   3679  O   MET B 887      16.716  -5.188 -29.170  1.00 44.83
ATOM   3680  CB  MET B 887      17.299  -4.525 -32.182  1.00 49.51
ATOM   3681  CG  MET B 887      16.366  -4.953 -33.287  1.00 52.27
ATOM   3682  SD  MET B 887      17.296  -5.341 -34.809  1.00 53.59
ATOM   3683  CE  MET B 887      17.031  -3.843 -35.775  1.00 56.07
ATOM   3684  N   ALA B 888      14.723  -4.785 -30.119  1.00 48.05
ATOM   3685  CA  ALA B 888      13.962  -5.683 -29.240  1.00 48.80
ATOM   3686  C   ALA B 888      14.288  -7.110 -29.661  1.00 49.42
ATOM   3687  O   ALA B 888      14.361  -7.406 -30.856  1.00 49.12
ATOM   3688  CB  ALA B 888      12.460  -5.432 -29.386  1.00 47.59
ATOM   3689  N   LEU B 889      14.472  -7.988 -28.681  1.00 50.17
ATOM   3690  CA  LEU B 889      14.829  -9.376 -28.941  1.00 51.55
ATOM   3691  C   LEU B 889      14.145 -10.030 -30.124  1.00 53.37
ATOM   3692  O   LEU B 889      14.806 -10.463 -31.076  1.00 54.40
ATOM   3693  CB  LEU B 889      14.570 -10.230 -27.713  1.00 52.02
ATOM   3694  CG  LEU B 889      14.987 -11.690 -27.885  1.00 53.15
ATOM   3695  CD1 LEU B 889      16.443 -11.748 -28.320  1.00 52.50
ATOM   3696  CD2 LEU B 889      14.777 -12.445 -26.571  1.00 52.22
ATOM   3697  N   GLU B 890      12.822 -10.114 -30.067  1.00 53.20
ATOM   3698  CA  GLU B 890      12.079 -10.745 -31.146  1.00 54.27
ATOM   3699  C   GLU B 890      12.498 -10.227 -32.521  1.00 55.82
ATOM   3700  O   GLU B 890      12.562 -10.994 -33.480  1.00 57.28
ATOM   3701  CB  GLU B 890      10.566 -10.557 -30.955  1.00 52.93
ATOM   3702  CG  GLU B 890      10.094  -9.116 -31.001  1.00 50.27
ATOM   3703  CD  GLU B 890      10.080  -8.445 -29.634  1.00 48.34
ATOM   3704  OE1 GLU B 890      10.893  -8.842 -28.759  1.00 44.27
ATOM   3705  OE2 GLU B 890       9.260  -7.509 -29.453  1.00 42.51
ATOM   3706  N   CYS B 891      12.798  -8.935 -32.613  1.00 57.27
ATOM   3707  CA  CYS B 891      13.192  -8.336 -33.888  1.00 58.36
ATOM   3708  C   CYS B 891      14.617  -8.642 -34.313  1.00 58.40
ATOM   3709  O   CYS B 891      15.052  -8.274 -35.401  1.00 56.71
ATOM   3710  CB  CYS B 891      12.972  -6.826 -33.852  1.00 59.30
ATOM   3711  SG  CYS B 891      11.232  -6.370 -33.986  1.00 58.60
ATOM   3712  N   ILE B 892      15.352  -9.324 -33.457  1.00 59.69
ATOM   3713  CA  ILE B 892      16.708  -9.677 -33.812  1.00 60.78
ATOM   3714  C   ILE B 892      16.692 -10.959 -34.647  1.00 60.92
ATOM   3715  O   ILE B 892      17.492 -11.104 -35.556  1.00 61.20
ATOM   3716  CB  ILE B 892      17.584  -9.872 -32.549  1.00 60.34
ATOM   3717  CG1 ILE B 892      17.844  -8.516 -31.898  1.00 59.88
ATOM   3718  CG2 ILE B 892      18.892 -10.551 -32.910  1.00 58.41
ATOM   3719  CD1 ILE B 892      18.713  -8.585 -30.683  1.00 61.44
ATOM   3720  N   HIS B 893      15.766 -11.873 -34.350  1.00 61.38
ATOM   3721  CA  HIS B 893      15.676 -13.143 -35.071  1.00 60.14
ATOM   3722  C   HIS B 893      14.811 -13.131 -36.329  1.00 57.92
```

```
ATOM   3723  O   HIS B 893      15.010 -13.940 -37.232  1.00 56.94
ATOM   3724  CB  HIS B 893      15.195 -14.245 -34.127  1.00 61.71
ATOM   3725  CG  HIS B 893      16.205 -14.626 -33.092  1.00 65.26
ATOM   3726  ND1 HIS B 893      17.326 -15.375 -33.384  1.00 66.05
ATOM   3727  CD2 HIS B 893      16.239 -14.400 -31.756  1.00 65.76
ATOM   3728  CE1 HIS B 893      18.006 -15.596 -32.272  1.00 66.79
ATOM   3729  NE2 HIS B 893      17.368 -15.016 -31.270  1.00 67.66
ATOM   3730  N   TYR B 894      13.850 -12.218 -36.379  1.00 55.44
ATOM   3731  CA  TYR B 894      12.956 -12.082 -37.523  1.00 53.67
ATOM   3732  C   TYR B 894      12.491 -10.649 -37.482  1.00 52.79
ATOM   3733  O   TYR B 894      12.909  -9.893 -36.620  1.00 53.67
ATOM   3734  CB  TYR B 894      11.738 -13.000 -37.387  1.00 53.49
ATOM   3735  CG  TYR B 894      12.051 -14.469 -37.473  1.00 54.03
ATOM   3736  CD1 TYR B 894      12.231 -15.091 -38.706  1.00 54.75
ATOM   3737  CD2 TYR B 894      12.223 -15.228 -36.318  1.00 55.06
ATOM   3738  CE1 TYR B 894      12.580 -16.438 -38.784  1.00 57.69
ATOM   3739  CE2 TYR B 894      12.574 -16.571 -36.381  1.00 57.19
ATOM   3740  CZ  TYR B 894      12.755 -17.175 -37.616  1.00 59.22
ATOM   3741  OH  TYR B 894      13.136 -18.504 -37.679  1.00 61.11
ATOM   3742  N   ARG B 895      11.623 -10.269 -38.405  1.00 53.26
ATOM   3743  CA  ARG B 895      11.112  -8.912 -38.417  1.00 53.71
ATOM   3744  C   ARG B 895       9.726  -8.838 -37.788  1.00 55.40
ATOM   3745  O   ARG B 895       8.700  -8.972 -38.464  1.00 56.92
ATOM   3746  CB  ARG B 895      11.066  -8.363 -39.840  1.00 52.60
ATOM   3747  CG  ARG B 895      12.425  -8.042 -40.416  1.00 54.61
ATOM   3748  CD  ARG B 895      12.326  -6.918 -41.439  1.00 56.13
ATOM   3749  NE  ARG B 895      13.641  -6.505 -41.914  1.00 58.90
ATOM   3750  CZ  ARG B 895      14.368  -7.200 -42.781  1.00 61.14
ATOM   3751  NH1 ARG B 895      13.894  -8.343 -43.271  1.00 61.94
ATOM   3752  NH2 ARG B 895      15.571  -6.767 -43.144  1.00 58.94
ATOM   3753  N   ALA B 896       9.705  -8.634 -36.476  1.00 55.24
ATOM   3754  CA  ALA B 896       8.452  -8.519 -35.748  1.00 53.33
ATOM   3755  C   ALA B 896       8.350  -7.085 -35.215  1.00 51.36
ATOM   3756  O   ALA B 896       8.063  -6.872 -34.040  1.00 51.66
ATOM   3757  CB  ALA B 896       8.419  -9.536 -34.598  1.00 52.72
ATOM   3758  N   PHE B 897       8.592  -6.104 -36.086  1.00 48.95
ATOM   3759  CA  PHE B 897       8.535  -4.695 -35.683  1.00 46.93
ATOM   3760  C   PHE B 897       7.134  -4.237 -35.300  1.00 44.17
ATOM   3761  O   PHE B 897       6.209  -4.266 -36.106  1.00 42.11
ATOM   3762  CB  PHE B 897       9.093  -3.785 -36.787  1.00 47.63
ATOM   3763  CG  PHE B 897      10.572  -3.928 -36.993  1.00 50.51
ATOM   3764  CD1 PHE B 897      11.076  -4.474 -38.172  1.00 53.25
ATOM   3765  CD2 PHE B 897      11.465  -3.567 -35.988  1.00 50.87
ATOM   3766  CE1 PHE B 897      12.451  -4.662 -38.342  1.00 52.04
ATOM   3767  CE2 PHE B 897      12.835  -3.750 -36.148  1.00 50.84
```

```
ATOM   3768  CZ  PHE B 897      13.329  -4.300 -37.326  1.00 52.35
ATOM   3769  N   THR B 898       6.997  -3.798 -34.055  1.00 42.52
ATOM   3770  CA  THR B 898       5.717  -3.352 -33.534  1.00 40.56
ATOM   3771  C   THR B 898       5.916  -2.231 -32.543  1.00 39.82
ATOM   3772  O   THR B 898       7.027  -1.983 -32.089  1.00 38.49
ATOM   3773  CB  THR B 898       5.000  -4.480 -32.779  1.00 39.38
ATOM   3774  OG1 THR B 898       5.744  -4.803 -31.602  1.00 39.33
ATOM   3775  CG2 THR B 898       4.881  -5.711 -33.638  1.00 37.90
ATOM   3776  N   HIS B 899       4.826  -1.558 -32.198  1.00 39.68
ATOM   3777  CA  HIS B 899       4.907  -0.487 -31.225  1.00 40.57
ATOM   3778  C   HIS B 899       5.672  -0.985 -29.998  1.00 39.75
ATOM   3779  O   HIS B 899       6.494  -0.262 -29.433  1.00 40.90
ATOM   3780  CB  HIS B 899       3.499  -0.040 -30.838  1.00 41.77
ATOM   3781  CG  HIS B 899       2.711   0.476 -31.994  1.00 44.38
ATOM   3782  ND1 HIS B 899       3.136   1.539 -32.765  1.00 46.58
ATOM   3783  CD2 HIS B 899       1.560   0.042 -32.554  1.00 44.66
ATOM   3784  CE1 HIS B 899       2.283   1.734 -33.752  1.00 45.15
ATOM   3785  NE2 HIS B 899       1.317   0.838 -33.648  1.00 47.56
ATOM   3786  N   GLN B 900       5.420  -2.227 -29.604  1.00 37.28
ATOM   3787  CA  GLN B 900       6.100  -2.770 -28.452  1.00 38.27
ATOM   3788  C   GLN B 900       7.608  -2.902 -28.658  1.00 38.64
ATOM   3789  O   GLN B 900       8.374  -2.701 -27.717  1.00 39.27
ATOM   3790  CB  GLN B 900       5.492  -4.112 -28.045  1.00 38.52
ATOM   3791  CG  GLN B 900       4.165  -3.987 -27.302  1.00 39.82
ATOM   3792  CD  GLN B 900       4.050  -2.696 -26.472  1.00 43.54
ATOM   3793  OE1 GLN B 900       3.859  -1.614 -27.025  1.00 46.46
ATOM   3794  NE2 GLN B 900       4.161  -2.812 -25.145  1.00 44.27
ATOM   3795  N   SER B 901       8.048  -3.226 -29.872  1.00 36.36
ATOM   3796  CA  SER B 901       9.482  -3.340 -30.110  1.00 35.93
ATOM   3797  C   SER B 901      10.093  -1.938 -30.014  1.00 37.71
ATOM   3798  O   SER B 901      11.239  -1.759 -29.584  1.00 35.11
ATOM   3799  CB  SER B 901       9.773  -3.993 -31.472  1.00 35.40
ATOM   3800  OG  SER B 901       9.213  -3.299 -32.566  1.00 35.60
ATOM   3801  N   ASP B 902       9.302  -0.936 -30.387  1.00 36.58
ATOM   3802  CA  ASP B 902       9.753   0.436 -30.297  1.00 35.05
ATOM   3803  C   ASP B 902       9.918   0.797 -28.816  1.00 35.23
ATOM   3804  O   ASP B 902      10.766   1.618 -28.453  1.00 31.03
ATOM   3805  CB  ASP B 902       8.738   1.368 -30.961  1.00 35.87
ATOM   3806  CG  ASP B 902       9.065   1.646 -32.421  1.00 38.00
ATOM   3807  OD1 ASP B 902      10.043   1.066 -32.944  1.00 35.01
ATOM   3808  OD2 ASP B 902       8.341   2.454 -33.043  1.00 40.53
ATOM   3809  N   VAL B 903       9.112   0.179 -27.957  1.00 34.13
ATOM   3810  CA  VAL B 903       9.214   0.479 -26.538  1.00 36.81
ATOM   3811  C   VAL B 903      10.559   0.008 -26.010  1.00 37.63
ATOM   3812  O   VAL B 903      11.184   0.674 -25.180  1.00 37.43
```

ATOM 3813 CB VAL B 903 8.075 -0.178 -25.727 1.00 38.45
ATOM 3814 CG1 VAL B 903 8.380 -0.100 -24.229 1.00 37.24
ATOM 3815 CG2 VAL B 903 6.763 0.533 -26.026 1.00 37.24
ATOM 3816 N TRP B 904 11.005 -1.144 -26.498 1.00 39.08
ATOM 3817 CA TRP B 904 12.297 -1.674 -26.092 1.00 37.59
ATOM 3818 C TRP B 904 13.332 -0.601 -26.441 1.00 34.67
ATOM 3819 O TRP B 904 14.129 -0.203 -25.602 1.00 32.68
ATOM 3820 CB TRP B 904 12.600 -2.980 -26.848 1.00 40.25
ATOM 3821 CG TRP B 904 13.943 -3.588 -26.523 1.00 41.50
ATOM 3822 CD1 TRP B 904 15.160 -3.031 -26.742 1.00 39.65
ATOM 3823 CD2 TRP B 904 14.190 -4.857 -25.891 1.00 43.17
ATOM 3824 NE1 TRP B 904 16.153 -3.861 -26.285 1.00 42.57
ATOM 3825 CE2 TRP B 904 15.588 -4.991 -25.759 1.00 43.45
ATOM 3826 CE3 TRP B 904 13.364 -5.892 -25.424 1.00 45.15
ATOM 3827 CZ2 TRP B 904 16.188 -6.123 -25.176 1.00 45.09
ATOM 3828 CZ3 TRP B 904 13.962 -7.024 -24.839 1.00 45.21
ATOM 3829 CH2 TRP B 904 15.360 -7.125 -24.724 1.00 44.37
ATOM 3830 N SER B 905 13.296 -0.123 -27.678 1.00 32.67
ATOM 3831 CA SER B 905 14.233 0.895 -28.120 1.00 34.81
ATOM 3832 C SER B 905 14.182 2.102 -27.190 1.00 35.70
ATOM 3833 O SER B 905 15.214 2.596 -26.727 1.00 35.81
ATOM 3834 CB SER B 905 13.904 1.309 -29.548 1.00 35.88
ATOM 3835 OG SER B 905 13.939 0.183 -30.404 1.00 34.89
ATOM 3836 N TYR B 906 12.963 2.556 -26.920 1.00 37.42
ATOM 3837 CA TYR B 906 12.712 3.679 -26.032 1.00 36.19
ATOM 3838 C TYR B 906 13.517 3.478 -24.763 1.00 36.71
ATOM 3839 O TYR B 906 14.208 4.378 -24.304 1.00 35.97
ATOM 3840 CB TYR B 906 11.226 3.741 -25.677 1.00 36.25
ATOM 3841 CG TYR B 906 10.889 4.865 -24.733 1.00 35.80
ATOM 3842 CD1 TYR B 906 10.571 6.130 -25.212 1.00 33.13
ATOM 3843 CD2 TYR B 906 10.983 4.683 -23.362 1.00 37.44
ATOM 3844 CE1 TYR B 906 10.369 7.183 -24.360 1.00 36.10
ATOM 3845 CE2 TYR B 906 10.782 5.738 -22.489 1.00 40.97
ATOM 3846 CZ TYR B 906 10.479 6.991 -22.994 1.00 39.58
ATOM 3847 OH TYR B 906 10.328 8.050 -22.125 1.00 39.67
ATOM 3848 N GLY B 907 13.409 2.289 -24.189 1.00 36.90
ATOM 3849 CA GLY B 907 14.150 1.995 -22.982 1.00 38.61
ATOM 3850 C GLY B 907 15.642 2.197 -23.171 1.00 41.80
ATOM 3851 O GLY B 907 16.285 2.870 -22.362 1.00 41.26
ATOM 3852 N VAL B 908 16.196 1.616 -24.238 1.00 43.21
ATOM 3853 CA VAL B 908 17.626 1.728 -24.527 1.00 42.16
ATOM 3854 C VAL B 908 17.967 3.191 -24.740 1.00 42.43
ATOM 3855 O VAL B 908 19.041 3.655 -24.358 1.00 42.57
ATOM 3856 CB VAL B 908 18.013 0.928 -25.794 1.00 43.20
ATOM 3857 CG1 VAL B 908 19.510 1.037 -26.052 1.00 42.14

```
ATOM   3858  CG2 VAL B 908      17.626  -0.525 -25.622  1.00 42.76
ATOM   3859  N   THR B 909      17.034   3.919 -25.338  1.00 40.59
ATOM   3860  CA  THR B 909      17.239   5.333 -25.583  1.00 40.05
ATOM   3861  C   THR B 909      17.318   6.168 -24.318  1.00 41.07
ATOM   3862  O   THR B 909      18.227   6.971 -24.180  1.00 44.18
ATOM   3863  CB  THR B 909      16.133   5.925 -26.447  1.00 38.19
ATOM   3864  OG1 THR B 909      16.119   5.268 -27.717  1.00 37.26
ATOM   3865  CG2 THR B 909      16.375   7.413 -26.658  1.00 35.17
ATOM   3866  N   ILE B 910      16.383   6.006 -23.390  1.00 41.77
ATOM   3867  CA  ILE B 910      16.459   6.830 -22.191  1.00 44.01
ATOM   3868  C   ILE B 910      17.678   6.440 -21.365  1.00 43.93
ATOM   3869  O   ILE B 910      18.162   7.222 -20.537  1.00 43.25
ATOM   3870  CB  ILE B 910      15.171   6.768 -21.323  1.00 44.35
ATOM   3871  CG1 ILE B 910      15.014   5.394 -20.688  1.00 45.86
ATOM   3872  CG2 ILE B 910      13.960   7.146 -22.179  1.00 44.14
ATOM   3873  CD1 ILE B 910      13.834   5.285 -19.766  1.00 45.31
ATOM   3874  N   TRP B 911      18.179   5.233 -21.611  1.00 43.13
ATOM   3875  CA  TRP B 911      19.369   4.746 -20.927  1.00 41.24
ATOM   3876  C   TRP B 911      20.542   5.605 -21.424  1.00 41.42
ATOM   3877  O   TRP B 911      21.375   6.032 -20.629  1.00 41.37
ATOM   3878  CB  TRP B 911      19.600   3.279 -21.265  1.00 42.93
ATOM   3879  CG  TRP B 911      20.768   2.671 -20.582  1.00 46.13
ATOM   3880  CD1 TRP B 911      20.778   2.044 -19.370  1.00 48.07
ATOM   3881  CD2 TRP B 911      22.120   2.647 -21.058  1.00 47.88
ATOM   3882  NE1 TRP B 911      22.053   1.629 -19.059  1.00 48.23
ATOM   3883  CE2 TRP B 911      22.897   1.988 -20.078  1.00 48.28
ATOM   3884  CE3 TRP B 911      22.751   3.123 -22.216  1.00 46.20
ATOM   3885  CZ2 TRP B 911      24.274   1.792 -20.221  1.00 45.73
ATOM   3886  CZ3 TRP B 911      24.120   2.928 -22.355  1.00 46.02
ATOM   3887  CH2 TRP B 911      24.865   2.268 -21.362  1.00 45.66
ATOM   3888  N   GLU B 912      20.600   5.874 -22.728  1.00 40.12
ATOM   3889  CA  GLU B 912      21.673   6.703 -23.263  1.00 42.28
ATOM   3890  C   GLU B 912      21.616   8.051 -22.573  1.00 43.95
ATOM   3891  O   GLU B 912      22.649   8.627 -22.228  1.00 45.55
ATOM   3892  CB  GLU B 912      21.524   6.955 -24.759  1.00 41.44
ATOM   3893  CG  GLU B 912      21.505   5.742 -25.635  1.00 44.81
ATOM   3894  CD  GLU B 912      21.220   6.107 -27.081  1.00 47.97
ATOM   3895  OE1 GLU B 912      22.153   6.551 -27.790  1.00 44.98
ATOM   3896  OE2 GLU B 912      20.049   5.964 -27.502  1.00 50.02
ATOM   3897  N   LEU B 913      20.402   8.558 -22.374  1.00 44.41
ATOM   3898  CA  LEU B 913      20.235   9.857 -21.734  1.00 43.18
ATOM   3899  C   LEU B 913      20.652   9.823 -20.270  1.00 43.99
ATOM   3900  O   LEU B 913      21.414  10.675 -19.823  1.00 44.57
ATOM   3901  CB  LEU B 913      18.787  10.332 -21.862  1.00 40.85
ATOM   3902  CG  LEU B 913      18.216  10.396 -23.286  1.00 41.67
```

ATOM 3903 CD1 LEU B 913 16.795 10.945 -23.221 1.00 39.11
ATOM 3904 CD2 LEU B 913 19.089 11.283 -24.187 1.00 38.24
ATOM 3905 N MET B 914 20.158 8.843 -19.519 1.00 45.82
ATOM 3906 CA MET B 914 20.513 8.742 -18.109 1.00 48.13
ATOM 3907 C MET B 914 22.023 8.596 -17.917 1.00 48.88
ATOM 3908 O MET B 914 22.553 8.972 -16.864 1.00 48.55
ATOM 3909 CB MET B 914 19.796 7.564 -17.443 1.00 50.82
ATOM 3910 CG MET B 914 18.292 7.740 -17.317 1.00 52.72
ATOM 3911 SD MET B 914 17.787 9.437 -16.952 1.00 53.52
ATOM 3912 CE MET B 914 16.626 9.705 -18.264 1.00 52.21
ATOM 3913 N THR B 915 22.710 8.048 -18.923 1.00 47.30
ATOM 3914 CA THR B 915 24.163 7.892 -18.849 1.00 46.63
ATOM 3915 C THR B 915 24.875 9.052 -19.562 1.00 48.58
ATOM 3916 O THR B 915 26.059 8.968 -19.886 1.00 48.03
ATOM 3917 CB THR B 915 24.642 6.559 -19.474 1.00 44.86
ATOM 3918 OG1 THR B 915 24.277 6.516 -20.860 1.00 44.85
ATOM 3919 CG2 THR B 915 24.043 5.373 -18.737 1.00 42.30
ATOM 3920 N PHE B 916 24.148 10.135 -19.809 1.00 50.49
ATOM 3921 CA PHE B 916 24.731 11.297 -20.463 1.00 52.07
ATOM 3922 C PHE B 916 25.505 10.901 -21.717 1.00 54.08
ATOM 3923 O PHE B 916 26.687 11.222 -21.848 1.00 56.00
ATOM 3924 CB PHE B 916 25.669 12.010 -19.489 1.00 52.26
ATOM 3925 CG PHE B 916 24.972 12.617 -18.305 1.00 52.03
ATOM 3926 CD1 PHE B 916 24.174 13.747 -18.452 1.00 52.39
ATOM 3927 CD2 PHE B 916 25.128 12.076 -17.040 1.00 52.11
ATOM 3928 CE1 PHE B 916 23.547 14.329 -17.356 1.00 51.26
ATOM 3929 CE2 PHE B 916 24.502 12.654 -15.938 1.00 52.35
ATOM 3930 CZ PHE B 916 23.713 13.781 -16.097 1.00 50.17
ATOM 3931 N GLY B 917 24.845 10.188 -22.626 1.00 54.77
ATOM 3932 CA GLY B 917 25.489 9.772 -23.863 1.00 53.58
ATOM 3933 C GLY B 917 26.130 8.392 -23.882 1.00 54.28
ATOM 3934 O GLY B 917 26.799 8.047 -24.858 1.00 56.32
ATOM 3935 N GLY B 918 25.925 7.596 -22.834 1.00 52.63
ATOM 3936 CA GLY B 918 26.519 6.268 -22.777 1.00 51.85
ATOM 3937 C GLY B 918 26.302 5.358 -23.977 1.00 53.07
ATOM 3938 O GLY B 918 25.357 5.533 -24.748 1.00 53.60
ATOM 3939 N LYS B 919 27.184 4.375 -24.136 1.00 53.42
ATOM 3940 CA LYS B 919 27.083 3.430 -25.241 1.00 53.94
ATOM 3941 C LYS B 919 26.529 2.081 -24.777 1.00 54.09
ATOM 3942 O LYS B 919 27.059 1.461 -23.853 1.00 53.78
ATOM 3943 CB LYS B 919 28.451 3.224 -25.898 1.00 56.15
ATOM 3944 CG LYS B 919 29.088 4.504 -26.440 1.00 60.22
ATOM 3945 CD LYS B 919 30.229 4.199 -27.399 1.00 62.11
ATOM 3946 CE LYS B 919 29.703 3.490 -28.644 1.00 65.81
ATOM 3947 NZ LYS B 919 30.785 3.065 -29.581 1.00 68.08

ATOM 3948 N PRO B 920 25.449 1.609 -25.424 1.00 53.96
ATOM 3949 CA PRO B 920 24.779 0.340 -25.122 1.00 52.93
ATOM 3950 C PRO B 920 25.730 -0.832 -25.235 1.00 52.53
ATOM 3951 O PRO B 920 26.390 -0.994 -26.254 1.00 51.03
ATOM 3952 CB PRO B 920 23.685 0.259 -26.184 1.00 52.25
ATOM 3953 CG PRO B 920 23.412 1.669 -26.510 1.00 54.01
ATOM 3954 CD PRO B 920 24.783 2.283 -26.550 1.00 53.55
ATOM 3955 N TYR B 921 25.774 -1.658 -24.197 1.00 54.38
ATOM 3956 CA TYR B 921 26.649 -2.823 -24.182 1.00 57.62
ATOM 3957 C TYR B 921 28.007 -2.445 -24.764 1.00 60.38
ATOM 3958 O TYR B 921 28.491 -3.075 -25.707 1.00 61.02
ATOM 3959 CB TYR B 921 26.022 -3.958 -24.992 1.00 56.19
ATOM 3960 CG TYR B 921 24.546 -4.115 -24.735 1.00 53.82
ATOM 3961 CD1 TYR B 921 23.612 -3.483 -25.551 1.00 54.08
ATOM 3962 CD2 TYR B 921 24.084 -4.862 -23.658 1.00 51.52
ATOM 3963 CE1 TYR B 921 22.257 -3.588 -25.303 1.00 53.70
ATOM 3964 CE2 TYR B 921 22.730 -4.975 -23.396 1.00 52.18
ATOM 3965 CZ TYR B 921 21.820 -4.337 -24.223 1.00 53.77
ATOM 3966 OH TYR B 921 20.474 -4.454 -23.983 1.00 52.26
ATOM 3967 N ASP B 922 28.605 -1.409 -24.184 1.00 63.62
ATOM 3968 CA ASP B 922 29.895 -0.888 -24.616 1.00 67.06
ATOM 3969 C ASP B 922 30.960 -1.967 -24.783 1.00 68.44
ATOM 3970 O ASP B 922 31.239 -2.732 -23.857 1.00 67.06
ATOM 3971 CB ASP B 922 30.400 0.152 -23.616 1.00 69.17
ATOM 3972 CG ASP B 922 31.481 1.037 -24.200 1.00 70.95
ATOM 3973 OD1 ASP B 922 32.337 0.521 -24.957 1.00 72.34
ATOM 3974 OD2 ASP B 922 31.478 2.250 -23.894 1.00 70.84
ATOM 3975 N GLY B 923 31.556 -2.008 -25.971 1.00 70.59
ATOM 3976 CA GLY B 923 32.595 -2.980 -26.257 1.00 72.18
ATOM 3977 C GLY B 923 32.100 -4.329 -26.747 1.00 72.53
ATOM 3978 O GLY B 923 32.580 -4.834 -27.759 1.00 74.13
ATOM 3979 N ILE B 924 31.142 -4.909 -26.032 1.00 71.67
ATOM 3980 CA ILE B 924 30.591 -6.215 -26.373 1.00 70.50
ATOM 3981 C ILE B 924 30.351 -6.414 -27.872 1.00 71.43
ATOM 3982 O ILE B 924 29.838 -5.527 -28.556 1.00 71.73
ATOM 3983 CB ILE B 924 29.278 -6.462 -25.597 1.00 69.48
ATOM 3984 CG1 ILE B 924 29.545 -6.319 -24.091 1.00 68.05
ATOM 3985 CG2 ILE B 924 28.729 -7.850 -25.917 1.00 67.40
ATOM 3986 CD1 ILE B 924 28.299 -6.301 -23.212 1.00 69.45
ATOM 3987 N PRO B 925 30.737 -7.594 -28.398 1.00 71.75
ATOM 3988 CA PRO B 925 30.619 -8.024 -29.799 1.00 71.06
ATOM 3989 C PRO B 925 29.197 -8.007 -30.368 1.00 69.91
ATOM 3990 O PRO B 925 28.333 -8.764 -29.935 1.00 68.95
ATOM 3991 CB PRO B 925 31.191 -9.442 -29.774 1.00 71.99
ATOM 3992 CG PRO B 925 32.182 -9.390 -28.661 1.00 72.05

```
ATOM   3993  CD  PRO B 925      31.432  -8.625 -27.604  1.00 72.02
ATOM   3994  N   THR B 926      28.977  -7.158 -31.361  1.00 69.43
ATOM   3995  CA  THR B 926      27.675  -7.030 -32.002  1.00 69.48
ATOM   3996  C   THR B 926      26.961  -8.380 -32.208  1.00 69.75
ATOM   3997  O   THR B 926      25.747  -8.486 -32.028  1.00 70.07
ATOM   3998  CB  THR B 926      27.826  -6.287 -33.366  1.00 70.00
ATOM   3999  OG1 THR B 926      26.543  -6.131 -33.980  1.00 68.48
ATOM   4000  CG2 THR B 926      28.766  -7.055 -34.309  1.00 70.72
ATOM   4001  N   ALA B 927      27.716  -9.412 -32.566  1.00 69.65
ATOM   4002  CA  ALA B 927      27.140 -10.732 -32.804  1.00 68.51
ATOM   4003  C   ALA B 927      26.683 -11.403 -31.510  1.00 68.30
ATOM   4004  O   ALA B 927      25.807 -12.270 -31.526  1.00 68.58
ATOM   4005  CB  ALA B 927      28.165 -11.626 -33.527  1.00 66.12
ATOM   4006  N   GLU B 928      27.272 -10.992 -30.392  1.00 68.00
ATOM   4007  CA  GLU B 928      26.958 -11.577 -29.090  1.00 68.38
ATOM   4008  C   GLU B 928      25.634 -11.170 -28.463  1.00 66.53
ATOM   4009  O   GLU B 928      25.007 -11.959 -27.753  1.00 64.89
ATOM   4010  CB  GLU B 928      28.075 -11.270 -28.088  1.00 71.51
ATOM   4011  CG  GLU B 928      29.263 -12.221 -28.136  1.00 75.50
ATOM   4012  CD  GLU B 928      30.041 -12.231 -26.826  1.00 79.00
ATOM   4013  OE1 GLU B 928      30.933 -13.095 -26.662  1.00 81.12
ATOM   4014  OE2 GLU B 928      29.760 -11.374 -25.957  1.00 79.77
ATOM   4015  N   ILE B 929      25.220  -9.936 -28.714  1.00 64.75
ATOM   4016  CA  ILE B 929      23.987  -9.415 -28.147  1.00 63.35
ATOM   4017  C   ILE B 929      22.858 -10.446 -28.077  1.00 63.03
ATOM   4018  O   ILE B 929      22.337 -10.734 -26.998  1.00 61.05
ATOM   4019  CB  ILE B 929      23.520  -8.184 -28.932  1.00 61.08
ATOM   4020  CG1 ILE B 929      24.652  -7.155 -28.994  1.00 58.47
ATOM   4021  CG2 ILE B 929      22.284  -7.600 -28.286  1.00 62.49
ATOM   4022  CD1 ILE B 929      25.199  -6.739 -27.651  1.00 53.78
ATOM   4023  N   PRO B 930      22.474 -11.026 -29.225  1.00 63.06
ATOM   4024  CA  PRO B 930      21.402 -12.024 -29.257  1.00 63.56
ATOM   4025  C   PRO B 930      21.495 -13.082 -28.155  1.00 64.62
ATOM   4026  O   PRO B 930      20.516 -13.350 -27.452  1.00 64.41
ATOM   4027  CB  PRO B 930      21.541 -12.617 -30.652  1.00 62.01
ATOM   4028  CG  PRO B 930      21.934 -11.428 -31.446  1.00 62.44
ATOM   4029  CD  PRO B 930      22.998 -10.792 -30.581  1.00 61.86
ATOM   4030  N   ASP B 931      22.668 -13.686 -28.004  1.00 65.47
ATOM   4031  CA  ASP B 931      22.839 -14.703 -26.982  1.00 66.27
ATOM   4032  C   ASP B 931      22.656 -14.072 -25.616  1.00 65.47
ATOM   4033  O   ASP B 931      21.839 -14.537 -24.821  1.00 64.75
ATOM   4034  CB  ASP B 931      24.227 -15.345 -27.078  1.00 70.06
ATOM   4035  CG  ASP B 931      24.483 -16.356 -25.967  1.00 73.85
ATOM   4036  OD1 ASP B 931      23.678 -17.313 -25.835  1.00 75.74
ATOM   4037  OD2 ASP B 931      25.484 -16.189 -25.228  1.00 74.15
```

```
ATOM   4038  N   LEU B 932      23.419 -13.011 -25.353  1.00 65.40
ATOM   4039  CA  LEU B 932      23.349 -12.298 -24.080  1.00 65.25
ATOM   4040  C   LEU B 932      21.902 -12.006 -23.678  1.00 65.94
ATOM   4041  O   LEU B 932      21.452 -12.390 -22.594  1.00 65.04
ATOM   4042  CB  LEU B 932      24.130 -10.982 -24.161  1.00 65.95
ATOM   4043  CG  LEU B 932      25.660 -11.055 -24.245  1.00 68.42
ATOM   4044  CD1 LEU B 932      26.237  -9.642 -24.271  1.00 69.04
ATOM   4045  CD2 LEU B 932      26.219 -11.823 -23.044  1.00 68.73
ATOM   4046  N   LEU B 933      21.173 -11.334 -24.562  1.00 65.07
ATOM   4047  CA  LEU B 933      19.787 -10.989 -24.298  1.00 64.62
ATOM   4048  C   LEU B 933      18.923 -12.152 -23.810  1.00 64.97
ATOM   4049  O   LEU B 933      18.110 -11.980 -22.899  1.00 65.95
ATOM   4050  CB  LEU B 933      19.166 -10.368 -25.548  1.00 63.72
ATOM   4051  CG  LEU B 933      19.756  -9.012 -25.939  1.00 63.23
ATOM   4052  CD1 LEU B 933      19.177  -8.570 -27.271  1.00 61.73
ATOM   4053  CD2 LEU B 933      19.464  -7.986 -24.852  1.00 61.35
ATOM   4054  N   GLU B 934      19.096 -13.331 -24.397  1.00 64.87
ATOM   4055  CA  GLU B 934      18.294 -14.487 -23.997  1.00 65.11
ATOM   4056  C   GLU B 934      18.805 -15.154 -22.730  1.00 63.75
ATOM   4057  O   GLU B 934      18.163 -16.050 -22.199  1.00 63.55
ATOM   4058  CB  GLU B 934      18.220 -15.494 -25.148  1.00 66.18
ATOM   4059  CG  GLU B 934      17.478 -14.925 -26.342  1.00 71.36
ATOM   4060  CD  GLU B 934      17.763 -15.642 -27.649  1.00 74.08
ATOM   4061  OE1 GLU B 934      18.950 -15.765 -28.029  1.00 75.67
ATOM   4062  OE2 GLU B 934      16.790 -16.066 -28.306  1.00 76.95
ATOM   4063  N   LYS B 935      19.958 -14.705 -22.249  1.00 63.26
ATOM   4064  CA  LYS B 935      20.558 -15.241 -21.032  1.00 63.78
ATOM   4065  C   LYS B 935      20.263 -14.297 -19.867  1.00 64.04
ATOM   4066  O   LYS B 935      20.830 -14.442 -18.783  1.00 65.10
ATOM   4067  CB  LYS B 935      22.077 -15.366 -21.185  1.00 64.14
ATOM   4068  CG  LYS B 935      22.556 -16.374 -22.206  1.00 65.76
ATOM   4069  CD  LYS B 935      22.334 -17.790 -21.719  1.00 68.99
ATOM   4070  CE  LYS B 935      23.035 -18.799 -22.610  1.00 70.04
ATOM   4071  NZ  LYS B 935      22.771 -20.184 -22.139  1.00 71.50
ATOM   4072  N   GLY B 936      19.406 -13.308 -20.105  1.00 62.82
ATOM   4073  CA  GLY B 936      19.055 -12.373 -19.051  1.00 61.39
ATOM   4074  C   GLY B 936      19.872 -11.097 -18.997  1.00 60.41
ATOM   4075  O   GLY B 936      19.600 -10.219 -18.185  1.00 60.95
ATOM   4076  N   GLU B 937      20.875 -10.987 -19.857  1.00 59.63
ATOM   4077  CA  GLU B 937      21.729  -9.797 -19.903  1.00 58.26
ATOM   4078  C   GLU B 937      20.903  -8.522 -20.150  1.00 56.06
ATOM   4079  O   GLU B 937      20.057  -8.496 -21.038  1.00 55.96
ATOM   4080  CB  GLU B 937      22.757  -9.958 -21.033  1.00 58.85
ATOM   4081  CG  GLU B 937      23.808  -8.877 -21.113  1.00 61.46
ATOM   4082  CD  GLU B 937      24.884  -9.045 -20.069  1.00 64.22
```

```
ATOM   4083  OE1 GLU B 937      25.719  -8.129 -19.921  1.00 66.78
ATOM   4084  OE2 GLU B 937      24.900 -10.099 -19.401  1.00 66.18
ATOM   4085  N   ARG B 938      21.135  -7.474 -19.366  1.00 53.07
ATOM   4086  CA  ARG B 938      20.427  -6.213 -19.567  1.00 51.85
ATOM   4087  C   ARG B 938      21.322  -5.046 -19.211  1.00 52.49
ATOM   4088  O   ARG B 938      22.249  -5.179 -18.405  1.00 54.14
ATOM   4089  CB  ARG B 938      19.154  -6.132 -18.728  1.00 49.08
ATOM   4090  CG  ARG B 938      18.047  -7.023 -19.212  1.00 48.98
ATOM   4091  CD  ARG B 938      17.653  -6.678 -20.629  1.00 51.23
ATOM   4092  NE  ARG B 938      17.145  -7.859 -21.322  1.00 56.53
ATOM   4093  CZ  ARG B 938      16.012  -8.471 -21.015  1.00 57.01
ATOM   4094  NH1 ARG B 938      15.267  -8.003 -20.025  1.00 62.70
ATOM   4095  NH2 ARG B 938      15.631  -9.549 -21.682  1.00 55.07
ATOM   4096  N   LEU B 939      21.043  -3.898 -19.813  1.00 50.95
ATOM   4097  CA  LEU B 939      21.832  -2.715 -19.547  1.00 51.34
ATOM   4098  C   LEU B 939      21.867  -2.401 -18.049  1.00 51.66
ATOM   4099  O   LEU B 939      20.869  -2.544 -17.343  1.00 50.27
ATOM   4100  CB  LEU B 939      21.282  -1.534 -20.349  1.00 49.96
ATOM   4101  CG  LEU B 939      21.558  -1.689 -21.849  1.00 49.98
ATOM   4102  CD1 LEU B 939      20.779  -0.666 -22.664  1.00 47.22
ATOM   4103  CD2 LEU B 939      23.050  -1.561 -22.078  1.00 47.98
ATOM   4104  N   PRO B 940      23.038  -1.976 -17.549  1.00 51.95
ATOM   4105  CA  PRO B 940      23.306  -1.620 -16.151  1.00 51.29
ATOM   4106  C   PRO B 940      22.397  -0.511 -15.667  1.00 51.06
ATOM   4107  O   PRO B 940      21.776   0.173 -16.469  1.00 52.57
ATOM   4108  CB  PRO B 940      24.751  -1.146 -16.184  1.00 50.42
ATOM   4109  CG  PRO B 940      25.325  -1.852 -17.362  1.00 52.89
ATOM   4110  CD  PRO B 940      24.233  -1.750 -18.376  1.00 50.94
ATOM   4111  N   GLN B 941      22.343  -0.324 -14.354  1.00 50.66
ATOM   4112  CA  GLN B 941      21.535   0.725 -13.760  1.00 48.49
ATOM   4113  C   GLN B 941      22.339   2.010 -13.777  1.00 46.91
ATOM   4114  O   GLN B 941      23.409   2.089 -13.200  1.00 47.29
ATOM   4115  CB  GLN B 941      21.151   0.357 -12.324  1.00 48.25
ATOM   4116  CG  GLN B 941      20.480   1.481 -11.554  1.00 49.45
ATOM   4117  CD  GLN B 941      19.811   1.011 -10.271  1.00 52.87
ATOM   4118  OE1 GLN B 941      19.261   1.815  -9.512  1.00 52.38
ATOM   4119  NE2 GLN B 941      19.842  -0.296 -10.026  1.00 55.49
ATOM   4120  N   PRO B 942      21.838   3.038 -14.460  1.00 48.21
ATOM   4121  CA  PRO B 942      22.613   4.278 -14.477  1.00 49.11
ATOM   4122  C   PRO B 942      22.849   4.807 -13.059  1.00 50.71
ATOM   4123  O   PRO B 942      21.954   4.803 -12.216  1.00 51.40
ATOM   4124  CB  PRO B 942      21.745   5.216 -15.315  1.00 46.82
ATOM   4125  CG  PRO B 942      21.020   4.271 -16.223  1.00 47.86
ATOM   4126  CD  PRO B 942      20.629   3.159 -15.289  1.00 45.98
ATOM   4127  N   PRO B 943      24.070   5.264 -12.782  1.00 51.83
```

ATOM 4128 CA PRO B 943 24.474 5.807 -11.484 1.00 51.12
ATOM 4129 C PRO B 943 23.470 6.802 -10.898 1.00 51.11
ATOM 4130 O PRO B 943 23.110 6.713 -9.723 1.00 51.29
ATOM 4131 CB PRO B 943 25.803 6.482 -11.805 1.00 52.65
ATOM 4132 CG PRO B 943 26.371 5.605 -12.856 1.00 52.13
ATOM 4133 CD PRO B 943 25.183 5.320 -13.744 1.00 52.53
ATOM 4134 N ILE B 944 23.028 7.748 -11.726 1.00 50.00
ATOM 4135 CA ILE B 944 22.099 8.792 -11.299 1.00 48.49
ATOM 4136 C ILE B 944 20.658 8.315 -11.174 1.00 49.21
ATOM 4137 O ILE B 944 19.785 9.043 -10.681 1.00 49.19
ATOM 4138 CB ILE B 944 22.117 9.983 -12.291 1.00 48.25
ATOM 4139 CG1 ILE B 944 21.350 9.618 -13.571 1.00 43.64
ATOM 4140 CG2 ILE B 944 23.557 10.345 -12.625 1.00 45.88
ATOM 4141 CD1 ILE B 944 21.185 10.768 -14.509 1.00 44.55
ATOM 4142 N CYS B 945 20.414 7.091 -11.623 1.00 49.20
ATOM 4143 CA CYS B 945 19.076 6.532 -11.595 1.00 50.25
ATOM 4144 C CYS B 945 18.623 6.005 -10.260 1.00 50.70
ATOM 4145 O CYS B 945 19.357 5.323 -9.553 1.00 53.59
ATOM 4146 CB CYS B 945 18.933 5.413 -12.630 1.00 50.33
ATOM 4147 SG CYS B 945 18.662 5.990 -14.307 1.00 50.97
ATOM 4148 N THR B 946 17.388 6.339 -9.930 1.00 49.35
ATOM 4149 CA THR B 946 16.765 5.883 -8.710 1.00 49.02
ATOM 4150 C THR B 946 16.161 4.554 -9.197 1.00 48.52
ATOM 4151 O THR B 946 15.777 4.457 -10.360 1.00 49.59
ATOM 4152 CB THR B 946 15.682 6.905 -8.282 1.00 46.42
ATOM 4153 OG1 THR B 946 15.473 6.829 -6.872 1.00 47.27
ATOM 4154 CG2 THR B 946 14.386 6.650 -9.002 1.00 43.71
ATOM 4155 N ILE B 947 16.100 3.527 -8.357 1.00 48.32
ATOM 4156 CA ILE B 947 15.546 2.252 -8.821 1.00 48.32
ATOM 4157 C ILE B 947 14.151 2.434 -9.422 1.00 48.84
ATOM 4158 O ILE B 947 13.685 1.600 -10.196 1.00 49.30
ATOM 4159 CB ILE B 947 15.478 1.180 -7.696 1.00 46.78
ATOM 4160 CG1 ILE B 947 15.096 -0.176 -8.312 1.00 49.09
ATOM 4161 CG2 ILE B 947 14.467 1.593 -6.627 1.00 46.28
ATOM 4162 CD1 ILE B 947 15.017 -1.363 -7.331 1.00 49.14
ATOM 4163 N ASP B 948 13.491 3.532 -9.075 1.00 49.00
ATOM 4164 CA ASP B 948 12.162 3.808 -9.611 1.00 50.27
ATOM 4165 C ASP B 948 12.247 3.963 -11.134 1.00 49.29
ATOM 4166 O ASP B 948 11.403 3.440 -11.874 1.00 48.74
ATOM 4167 CB ASP B 948 11.602 5.098 -9.002 1.00 53.06
ATOM 4168 CG ASP B 948 11.377 4.995 -7.503 1.00 53.88
ATOM 4169 OD1 ASP B 948 10.208 4.869 -7.094 1.00 54.68
ATOM 4170 OD2 ASP B 948 12.363 5.044 -6.736 1.00 55.07
ATOM 4171 N VAL B 949 13.272 4.691 -11.583 1.00 47.43
ATOM 4172 CA VAL B 949 13.515 4.940 -13.001 1.00 45.11

```
ATOM   4173  C   VAL B 949      14.030   3.686 -13.692  1.00 46.35
ATOM   4174  O   VAL B 949      13.546   3.304 -14.767  1.00 46.15
ATOM   4175  CB  VAL B 949      14.576   6.043 -13.208  1.00 44.06
ATOM   4176  CG1 VAL B 949      14.835   6.254 -14.696  1.00 41.72
ATOM   4177  CG2 VAL B 949      14.128   7.325 -12.565  1.00 40.72
ATOM   4178  N   TYR B 950      15.019   3.050 -13.068  1.00 46.25
ATOM   4179  CA  TYR B 950      15.613   1.850 -13.629  1.00 46.35
ATOM   4180  C   TYR B 950      14.590   0.760 -13.932  1.00 45.76
ATOM   4181  O   TYR B 950      14.665   0.122 -14.977  1.00 43.83
ATOM   4182  CB  TYR B 950      16.689   1.297 -12.694  1.00 46.54
ATOM   4183  CG  TYR B 950      17.528   0.203 -13.325  1.00 49.48
ATOM   4184  CD1 TYR B 950      18.209   0.422 -14.524  1.00 48.95
ATOM   4185  CD2 TYR B 950      17.649  -1.050 -12.721  1.00 51.79
ATOM   4186  CE1 TYR B 950      18.986  -0.571 -15.105  1.00 49.83
ATOM   4187  CE2 TYR B 950      18.428  -2.057 -13.294  1.00 51.29
ATOM   4188  CZ  TYR B 950      19.096  -1.809 -14.485  1.00 51.48
ATOM   4189  OH  TYR B 950      19.891  -2.785 -15.041  1.00 49.38
ATOM   4190  N   MET B 951      13.636   0.547 -13.030  1.00 46.47
ATOM   4191  CA  MET B 951      12.630  -0.484 -13.258  1.00 47.95
ATOM   4192  C   MET B 951      11.790  -0.156 -14.480  1.00 47.93
ATOM   4193  O   MET B 951      11.274  -1.059 -15.152  1.00 50.04
ATOM   4194  CB  MET B 951      11.741  -0.679 -12.026  1.00 49.33
ATOM   4195  CG  MET B 951      12.514  -1.169 -10.798  1.00 55.37
ATOM   4196  SD  MET B 951      13.753  -2.470 -11.188  1.00 62.22
ATOM   4197  CE  MET B 951      12.677  -3.817 -11.608  1.00 59.62
ATOM   4198  N   VAL B 952      11.650   1.128 -14.784  1.00 45.24
ATOM   4199  CA  VAL B 952      10.896   1.494 -15.971  1.00 44.94
ATOM   4200  C   VAL B 952      11.668   0.969 -17.194  1.00 44.46
ATOM   4201  O   VAL B 952      11.113   0.260 -18.037  1.00 42.31
ATOM   4202  CB  VAL B 952      10.694   3.031 -16.067  1.00 44.63
ATOM   4203  CG1 VAL B 952      10.122   3.407 -17.423  1.00 40.56
ATOM   4204  CG2 VAL B 952       9.738   3.489 -14.971  1.00 42.36
ATOM   4205  N   MET B 953      12.954   1.300 -17.269  1.00 44.54
ATOM   4206  CA  MET B 953      13.789   0.846 -18.377  1.00 45.71
ATOM   4207  C   MET B 953      13.760  -0.677 -18.498  1.00 45.34
ATOM   4208  O   MET B 953      13.606  -1.218 -19.598  1.00 44.65
ATOM   4209  CB  MET B 953      15.227   1.307 -18.179  1.00 46.83
ATOM   4210  CG  MET B 953      15.396   2.800 -18.224  1.00 52.42
ATOM   4211  SD  MET B 953      16.973   3.296 -17.565  1.00 57.82
ATOM   4212  CE  MET B 953      16.787   5.046 -17.587  1.00 57.27
ATOM   4213  N   VAL B 954      13.903  -1.365 -17.369  1.00 43.09
ATOM   4214  CA  VAL B 954      13.891  -2.815 -17.375  1.00 43.36
ATOM   4215  C   VAL B 954      12.588  -3.343 -17.961  1.00 43.58
ATOM   4216  O   VAL B 954      12.605  -4.189 -18.857  1.00 41.66
ATOM   4217  CB  VAL B 954      14.094  -3.379 -15.961  1.00 43.56
```

ATOM 4218 CG1 VAL B 954 14.037 -4.883 -15.993 1.00 45.22
ATOM 4219 CG2 VAL B 954 15.439 -2.946 -15.430 1.00 44.09
ATOM 4220 N LYS B 955 11.459 -2.827 -17.476 1.00 44.30
ATOM 4221 CA LYS B 955 10.158 -3.262 -17.982 1.00 44.82
ATOM 4222 C LYS B 955 10.096 -3.192 -19.504 1.00 44.68
ATOM 4223 O LYS B 955 9.542 -4.072 -20.160 1.00 46.69
ATOM 4224 CB LYS B 955 9.041 -2.410 -17.391 1.00 46.61
ATOM 4225 CG LYS B 955 8.647 -2.770 -15.972 1.00 46.76
ATOM 4226 CD LYS B 955 7.588 -1.812 -15.500 1.00 47.23
ATOM 4227 CE LYS B 955 7.121 -2.128 -14.119 1.00 48.72
ATOM 4228 NZ LYS B 955 6.636 -0.872 -13.502 1.00 52.38
ATOM 4229 N CYS B 956 10.665 -2.139 -20.066 1.00 43.75
ATOM 4230 CA CYS B 956 10.682 -1.978 -21.509 1.00 43.94
ATOM 4231 C CYS B 956 11.396 -3.138 -22.195 1.00 45.19
ATOM 4232 O CYS B 956 11.205 -3.365 -23.397 1.00 43.93
ATOM 4233 CB CYS B 956 11.410 -0.692 -21.883 1.00 42.14
ATOM 4234 SG CYS B 956 10.593 0.788 -21.373 1.00 41.02
ATOM 4235 N TRP B 957 12.221 -3.860 -21.433 1.00 44.92
ATOM 4236 CA TRP B 957 12.995 -4.957 -21.995 1.00 45.41
ATOM 4237 C TRP B 957 12.543 -6.352 -21.592 1.00 47.76
ATOM 4238 O TRP B 957 13.328 -7.295 -21.641 1.00 47.21
ATOM 4239 CB TRP B 957 14.477 -4.783 -21.645 1.00 41.77
ATOM 4240 CG TRP B 957 15.012 -3.417 -21.957 1.00 38.80
ATOM 4241 CD1 TRP B 957 14.764 -2.680 -23.074 1.00 38.90
ATOM 4242 CD2 TRP B 957 15.910 -2.633 -21.150 1.00 37.82
ATOM 4243 NE1 TRP B 957 15.444 -1.482 -23.019 1.00 39.19
ATOM 4244 CE2 TRP B 957 16.159 -1.429 -21.851 1.00 37.54
ATOM 4245 CE3 TRP B 957 16.528 -2.832 -19.907 1.00 36.20
ATOM 4246 CZ2 TRP B 957 17.004 -0.425 -21.353 1.00 36.54
ATOM 4247 CZ3 TRP B 957 17.366 -1.835 -19.414 1.00 39.57
ATOM 4248 CH2 TRP B 957 17.596 -0.643 -20.142 1.00 36.55
ATOM 4249 N MET B 958 11.289 -6.491 -21.185 1.00 49.98
ATOM 4250 CA MET B 958 10.793 -7.810 -20.828 1.00 50.86
ATOM 4251 C MET B 958 10.806 -8.612 -22.115 1.00 50.79
ATOM 4252 O MET B 958 10.734 -8.045 -23.205 1.00 49.90
ATOM 4253 CB MET B 958 9.373 -7.731 -20.264 1.00 52.90
ATOM 4254 CG MET B 958 9.295 -7.075 -18.896 1.00 55.44
ATOM 4255 SD MET B 958 10.524 -7.763 -17.765 1.00 57.70
ATOM 4256 CE MET B 958 9.531 -9.050 -16.941 1.00 59.85
ATOM 4257 N ILE B 959 10.914 -9.927 -21.998 1.00 51.99
ATOM 4258 CA ILE B 959 10.955 -10.768 -23.184 1.00 53.60
ATOM 4259 C ILE B 959 9.611 -10.696 -23.888 1.00 52.84
ATOM 4260 O ILE B 959 9.536 -10.632 -25.111 1.00 52.06
ATOM 4261 CB ILE B 959 11.251 -12.232 -22.823 1.00 55.50
ATOM 4262 CG1 ILE B 959 12.621 -12.335 -22.135 1.00 59.93

```
ATOM   4263  CG2 ILE B 959      11.235 -13.079 -24.090  1.00 56.33
ATOM   4264  CD1 ILE B 959      12.904 -13.710 -21.482  1.00 62.42
ATOM   4265  N   ASP B 960       8.551 -10.695 -23.093  1.00 53.61
ATOM   4266  CA  ASP B 960       7.192 -10.625 -23.610  1.00 54.49
ATOM   4267  C   ASP B 960       6.860  -9.199 -24.063  1.00 52.87
ATOM   4268  O   ASP B 960       6.711  -8.290 -23.250  1.00 50.14
ATOM   4269  CB  ASP B 960       6.212 -11.072 -22.528  1.00 57.08
ATOM   4270  CG  ASP B 960       4.851 -11.400 -23.081  1.00 61.48
ATOM   4271  OD1 ASP B 960       4.233 -10.509 -23.706  1.00 65.36
ATOM   4272  OD2 ASP B 960       4.395 -12.550 -22.891  1.00 64.23
ATOM   4273  N   ALA B 961       6.745  -9.020 -25.371  1.00 52.25
ATOM   4274  CA  ALA B 961       6.438  -7.722 -25.950  1.00 53.15
ATOM   4275  C   ALA B 961       5.192  -7.090 -25.339  1.00 54.47
ATOM   4276  O   ALA B 961       5.188  -5.902 -25.013  1.00 54.47
ATOM   4277  CB  ALA B 961       6.263  -7.864 -27.449  1.00 49.84
ATOM   4278  N   ASP B 962       4.140  -7.888 -25.182  1.00 56.23
ATOM   4279  CA  ASP B 962       2.888  -7.393 -24.618  1.00 57.94
ATOM   4280  C   ASP B 962       2.943  -7.036 -23.135  1.00 56.89
ATOM   4281  O   ASP B 962       2.045  -6.358 -22.632  1.00 57.51
ATOM   4282  CB  ASP B 962       1.748  -8.396 -24.840  1.00 60.84
ATOM   4283  CG  ASP B 962       1.280  -8.451 -26.289  1.00 64.87
ATOM   4284  OD1 ASP B 962       1.123  -7.376 -26.915  1.00 66.69
ATOM   4285  OD2 ASP B 962       1.054  -9.575 -26.794  1.00 67.24
ATOM   4286  N   SER B 963       3.973  -7.481 -22.422  1.00 54.15
ATOM   4287  CA  SER B 963       4.050  -7.144 -21.008  1.00 52.47
ATOM   4288  C   SER B 963       4.973  -5.954 -20.761  1.00 50.73
ATOM   4289  O   SER B 963       5.319  -5.646 -19.623  1.00 51.91
ATOM   4290  CB  SER B 963       4.502  -8.354 -20.188  1.00 53.91
ATOM   4291  OG  SER B 963       5.814  -8.753 -20.531  1.00 56.30
ATOM   4292  N   ARG B 964       5.380  -5.288 -21.835  1.00 48.87
ATOM   4293  CA  ARG B 964       6.235  -4.115 -21.710  1.00 47.43
ATOM   4294  C   ARG B 964       5.327  -2.916 -21.536  1.00 45.64
ATOM   4295  O   ARG B 964       4.202  -2.898 -22.036  1.00 46.22
ATOM   4296  CB  ARG B 964       7.079  -3.914 -22.964  1.00 46.37
ATOM   4297  CG  ARG B 964       8.058  -5.025 -23.230  1.00 47.48
ATOM   4298  CD  ARG B 964       8.697  -4.888 -24.604  1.00 46.80
ATOM   4299  NE  ARG B 964       9.474  -6.074 -24.930  1.00 47.04
ATOM   4300  CZ  ARG B 964       9.889  -6.388 -26.149  1.00 46.77
ATOM   4301  NH1 ARG B 964       9.609  -5.600 -27.174  1.00 46.76
ATOM   4302  NH2 ARG B 964      10.564  -7.507 -26.343  1.00 48.41
ATOM   4303  N   PRO B 965       5.800  -1.890 -20.831  1.00 43.80
ATOM   4304  CA  PRO B 965       4.915  -0.733 -20.671  1.00 43.62
ATOM   4305  C   PRO B 965       4.533  -0.150 -22.022  1.00 42.50
ATOM   4306  O   PRO B 965       5.260  -0.301 -23.005  1.00 43.40
ATOM   4307  CB  PRO B 965       5.743   0.226 -19.821  1.00 42.89
```

ATOM 4308 CG PRO B 965 7.161 -0.156 -20.152 1.00 45.29
ATOM 4309 CD PRO B 965 7.122 -1.653 -20.233 1.00 43.22
ATOM 4310 N LYS B 966 3.373 0.490 -22.080 1.00 40.83
ATOM 4311 CA LYS B 966 2.932 1.102 -23.313 1.00 40.21
ATOM 4312 C LYS B 966 3.289 2.583 -23.303 1.00 39.83
ATOM 4313 O LYS B 966 3.423 3.189 -22.232 1.00 38.40
ATOM 4314 CB LYS B 966 1.446 0.861 -23.491 1.00 41.77
ATOM 4315 CG LYS B 966 1.194 -0.588 -23.796 1.00 47.30
ATOM 4316 CD LYS B 966 -0.223 -0.888 -24.170 1.00 51.96
ATOM 4317 CE LYS B 966 -0.392 -2.395 -24.327 1.00 57.53
ATOM 4318 NZ LYS B 966 -1.831 -2.804 -24.235 1.00 61.18
ATOM 4319 N PHE B 967 3.469 3.167 -24.485 1.00 38.02
ATOM 4320 CA PHE B 967 3.866 4.569 -24.547 1.00 40.61
ATOM 4321 C PHE B 967 2.998 5.514 -23.741 1.00 41.52
ATOM 4322 O PHE B 967 3.509 6.479 -23.180 1.00 42.24
ATOM 4323 CB PHE B 967 4.007 5.032 -26.004 1.00 38.99
ATOM 4324 CG PHE B 967 5.289 4.572 -26.648 1.00 38.22
ATOM 4325 CD1 PHE B 967 5.279 3.891 -27.858 1.00 37.36
ATOM 4326 CD2 PHE B 967 6.510 4.769 -26.002 1.00 37.25
ATOM 4327 CE1 PHE B 967 6.477 3.405 -28.417 1.00 42.23
ATOM 4328 CE2 PHE B 967 7.712 4.287 -26.551 1.00 39.11
ATOM 4329 CZ PHE B 967 7.698 3.605 -27.756 1.00 39.07
ATOM 4330 N ALA B 968 1.701 5.223 -23.652 1.00 42.04
ATOM 4331 CA ALA B 968 0.792 6.059 -22.872 1.00 44.04
ATOM 4332 C ALA B 968 1.210 6.066 -21.398 1.00 46.45
ATOM 4333 O ALA B 968 1.146 7.098 -20.729 1.00 46.84
ATOM 4334 CB ALA B 968 -0.650 5.549 -22.998 1.00 42.69
ATOM 4335 N GLU B 969 1.640 4.913 -20.895 1.00 46.92
ATOM 4336 CA GLU B 969 2.048 4.804 -19.503 1.00 47.61
ATOM 4337 C GLU B 969 3.420 5.396 -19.227 1.00 47.48
ATOM 4338 O GLU B 969 3.637 6.015 -18.182 1.00 47.99
ATOM 4339 CB GLU B 969 2.079 3.349 -19.065 1.00 51.22
ATOM 4340 CG GLU B 969 0.851 2.539 -19.384 1.00 57.69
ATOM 4341 CD GLU B 969 1.087 1.070 -19.086 1.00 62.44
ATOM 4342 OE1 GLU B 969 1.928 0.442 -19.771 1.00 63.17
ATOM 4343 OE2 GLU B 969 0.446 0.546 -18.151 1.00 68.35
ATOM 4344 N LEU B 970 4.362 5.182 -20.138 1.00 45.82
ATOM 4345 CA LEU B 970 5.699 5.704 -19.917 1.00 44.09
ATOM 4346 C LEU B 970 5.597 7.211 -19.807 1.00 44.59
ATOM 4347 O LEU B 970 6.152 7.819 -18.890 1.00 45.03
ATOM 4348 CB LEU B 970 6.645 5.276 -21.050 1.00 43.43
ATOM 4349 CG LEU B 970 7.053 3.782 -21.016 1.00 43.26
ATOM 4350 CD1 LEU B 970 7.660 3.340 -22.331 1.00 40.75
ATOM 4351 CD2 LEU B 970 8.029 3.551 -19.887 1.00 40.19
ATOM 4352 N ALA B 971 4.849 7.815 -20.718 1.00 44.94

ATOM 4353 CA ALA B 971 4.684 9.257 -20.690 1.00 45.01
ATOM 4354 C ALA B 971 4.093 9.663 -19.350 1.00 46.07
ATOM 4355 O ALA B 971 4.559 10.602 -18.709 1.00 48.26
ATOM 4356 CB ALA B 971 3.782 9.699 -21.806 1.00 43.14
ATOM 4357 N ALA B 972 3.075 8.939 -18.919 1.00 43.91
ATOM 4358 CA ALA B 972 2.435 9.242 -17.660 1.00 46.47
ATOM 4359 C ALA B 972 3.386 9.110 -16.466 1.00 48.41
ATOM 4360 O ALA B 972 3.481 10.018 -15.635 1.00 50.02
ATOM 4361 CB ALA B 972 1.233 8.339 -17.474 1.00 46.27
ATOM 4362 N GLU B 973 4.092 7.988 -16.377 1.00 49.34
ATOM 4363 CA GLU B 973 5.003 7.768 -15.259 1.00 50.14
ATOM 4364 C GLU B 973 6.160 8.769 -15.233 1.00 49.00
ATOM 4365 O GLU B 973 6.488 9.309 -14.182 1.00 47.51
ATOM 4366 CB GLU B 973 5.537 6.330 -15.295 1.00 53.73
ATOM 4367 CG GLU B 973 6.424 5.917 -14.120 1.00 58.85
ATOM 4368 CD GLU B 973 5.733 6.039 -12.764 1.00 64.87
ATOM 4369 OE1 GLU B 973 4.555 5.625 -12.644 1.00 67.25
ATOM 4370 OE2 GLU B 973 6.374 6.540 -11.808 1.00 67.54
ATOM 4371 N PHE B 974 6.784 9.026 -16.376 1.00 47.15
ATOM 4372 CA PHE B 974 7.892 9.970 -16.385 1.00 46.71
ATOM 4373 C PHE B 974 7.340 11.351 -16.178 1.00 47.30
ATOM 4374 O PHE B 974 8.017 12.242 -15.672 1.00 45.15
ATOM 4375 CB PHE B 974 8.649 9.898 -17.700 1.00 44.76
ATOM 4376 CG PHE B 974 9.648 8.794 -17.742 1.00 45.39
ATOM 4377 CD1 PHE B 974 10.790 8.851 -16.952 1.00 43.84
ATOM 4378 CD2 PHE B 974 9.433 7.669 -18.533 1.00 44.99
ATOM 4379 CE1 PHE B 974 11.705 7.800 -16.946 1.00 43.56
ATOM 4380 CE2 PHE B 974 10.343 6.612 -18.531 1.00 44.73
ATOM 4381 CZ PHE B 974 11.480 6.680 -17.734 1.00 43.10
ATOM 4382 N SER B 975 6.082 11.509 -16.564 1.00 48.14
ATOM 4383 CA SER B 975 5.393 12.775 -16.427 1.00 48.35
ATOM 4384 C SER B 975 5.302 13.184 -14.953 1.00 48.95
ATOM 4385 O SER B 975 5.666 14.305 -14.589 1.00 49.88
ATOM 4386 CB SER B 975 3.999 12.661 -17.040 1.00 48.77
ATOM 4387 OG SER B 975 3.325 13.899 -17.030 1.00 52.34
ATOM 4388 N ARG B 976 4.831 12.287 -14.093 1.00 47.45
ATOM 4389 CA ARG B 976 4.732 12.658 -12.697 1.00 47.19
ATOM 4390 C ARG B 976 6.105 12.708 -12.029 1.00 47.91
ATOM 4391 O ARG B 976 6.298 13.433 -11.055 1.00 48.07
ATOM 4392 CB ARG B 976 3.771 11.721 -11.942 1.00 47.00
ATOM 4393 CG ARG B 976 4.268 10.343 -11.695 1.00 48.59
ATOM 4394 CD ARG B 976 3.392 9.578 -10.696 1.00 51.30
ATOM 4395 NE ARG B 976 4.049 8.319 -10.349 1.00 53.72
ATOM 4396 CZ ARG B 976 5.139 8.240 -9.593 1.00 56.06
ATOM 4397 NH1 ARG B 976 5.697 7.066 -9.337 1.00 58.55

```
ATOM   4398  NH2 ARG B 976       5.652   9.337  -9.056  1.00 57.80
ATOM   4399  N   MET B 977       7.065  11.960 -12.558  1.00 49.05
ATOM   4400  CA  MET B 977       8.407  11.967 -11.988  1.00 51.32
ATOM   4401  C   MET B 977       9.021  13.332 -12.249  1.00 52.43
ATOM   4402  O   MET B 977       9.887  13.796 -11.503  1.00 52.50
ATOM   4403  CB  MET B 977       9.269  10.854 -12.604  1.00 52.10
ATOM   4404  CG  MET B 977       9.056   9.489 -11.939  1.00 54.48
ATOM   4405  SD  MET B 977       9.708   8.090 -12.871  1.00 54.18
ATOM   4406  CE  MET B 977      11.338   8.258 -12.532  1.00 54.40
ATOM   4407  N   ALA B 978       8.548  13.981 -13.309  1.00 53.20
ATOM   4408  CA  ALA B 978       9.030  15.303 -13.672  1.00 52.59
ATOM   4409  C   ALA B 978       8.429  16.332 -12.714  1.00 53.53
ATOM   4410  O   ALA B 978       8.910  17.468 -12.625  1.00 53.68
ATOM   4411  CB  ALA B 978       8.647  15.621 -15.112  1.00 49.91
ATOM   4412  N   ARG B 979       7.379  15.936 -11.999  1.00 53.98
ATOM   4413  CA  ARG B 979       6.749  16.836 -11.042  1.00 57.90
ATOM   4414  C   ARG B 979       7.590  16.920  -9.767  1.00 59.18
ATOM   4415  O   ARG B 979       7.417  17.834  -8.970  1.00 61.14
ATOM   4416  CB  ARG B 979       5.329  16.367 -10.704  1.00 59.68
ATOM   4417  CG  ARG B 979       4.322  16.484 -11.856  1.00 61.54
ATOM   4418  CD  ARG B 979       3.022  15.725 -11.544  1.00 61.64
ATOM   4419  NE  ARG B 979       2.376  15.243 -12.766  1.00 63.13
ATOM   4420  CZ  ARG B 979       1.427  14.309 -12.809  1.00 62.83
ATOM   4421  NH1 ARG B 979       0.989  13.740 -11.690  1.00 63.57
ATOM   4422  NH2 ARG B 979       0.931  13.924 -13.980  1.00 62.38
ATOM   4423  N   ASP B 980       8.496  15.964  -9.583  1.00 59.01
ATOM   4424  CA  ASP B 980       9.384  15.936  -8.422  1.00 59.63
ATOM   4425  C   ASP B 980      10.685  15.245  -8.872  1.00 60.07
ATOM   4426  O   ASP B 980      11.062  14.183  -8.362  1.00 58.65
ATOM   4427  CB  ASP B 980       8.709  15.177  -7.262  1.00 60.54
ATOM   4428  CG  ASP B 980       9.456  15.334  -5.922  1.00 62.11
ATOM   4429  OD1 ASP B 980      10.255  16.288  -5.765  1.00 61.29
ATOM   4430  OD2 ASP B 980       9.226  14.502  -5.015  1.00 61.48
ATOM   4431  N   PRO B 981      11.392  15.865  -9.837  1.00 59.64
ATOM   4432  CA  PRO B 981      12.651  15.412 -10.445  1.00 60.15
ATOM   4433  C   PRO B 981      13.831  14.975  -9.573  1.00 60.53
ATOM   4434  O   PRO B 981      14.609  14.114  -9.986  1.00 60.77
ATOM   4435  CB  PRO B 981      13.025  16.574 -11.372  1.00 58.58
ATOM   4436  CG  PRO B 981      12.393  17.753 -10.726  1.00 57.47
ATOM   4437  CD  PRO B 981      11.049  17.213 -10.331  1.00 58.74
ATOM   4438  N   GLN B 982      13.981  15.558  -8.386  1.00 61.15
ATOM   4439  CA  GLN B 982      15.102  15.197  -7.521  1.00 60.07
ATOM   4440  C   GLN B 982      14.854  13.919  -6.745  1.00 57.60
ATOM   4441  O   GLN B 982      15.774  13.355  -6.167  1.00 56.36
ATOM   4442  CB  GLN B 982      15.427  16.339  -6.559  1.00 63.51
```

```
ATOM   4443  CG  GLN B 982      16.078  17.547  -7.228  1.00 66.46
ATOM   4444  CD  GLN B 982      16.277  18.713  -6.272  1.00 69.16
ATOM   4445  OE1 GLN B 982      15.811  18.681  -5.134  1.00 72.71
ATOM   4446  NE2 GLN B 982      16.977  19.745  -6.729  1.00 70.65
ATOM   4447  N   ARG B 983      13.607  13.464  -6.745  1.00 56.49
ATOM   4448  CA  ARG B 983      13.221  12.230  -6.062  1.00 54.51
ATOM   4449  C   ARG B 983      13.456  11.011  -6.955  1.00 52.63
ATOM   4450  O   ARG B 983      13.445   9.870  -6.489  1.00 51.88
ATOM   4451  CB  ARG B 983      11.741  12.280  -5.693  1.00 54.81
ATOM   4452  CG  ARG B 983      11.219  11.016  -5.031  1.00 56.29
ATOM   4453  CD  ARG B 983       9.712  11.054  -4.892  1.00 57.50
ATOM   4454  NE  ARG B 983       9.214   9.997  -4.018  1.00 58.23
ATOM   4455  CZ  ARG B 983       7.924   9.735  -3.834  1.00 57.38
ATOM   4456  NH1 ARG B 983       7.003  10.452  -4.469  1.00 56.60
ATOM   4457  NH2 ARG B 983       7.556   8.765  -3.011  1.00 57.50
ATOM   4458  N   TYR B 984      13.673  11.257  -8.241  1.00 50.73
ATOM   4459  CA  TYR B 984      13.874  10.166  -9.172  1.00 50.45
ATOM   4460  C   TYR B 984      15.240  10.063  -9.855  1.00 48.61
ATOM   4461  O   TYR B 984      15.605   8.994 -10.339  1.00 48.45
ATOM   4462  CB  TYR B 984      12.724  10.175 -10.177  1.00 49.68
ATOM   4463  CG  TYR B 984      11.415   9.906  -9.468  1.00 53.31
ATOM   4464  CD1 TYR B 984      10.591  10.950  -9.047  1.00 54.83
ATOM   4465  CD2 TYR B 984      11.049   8.606  -9.118  1.00 54.60
ATOM   4466  CE1 TYR B 984       9.435  10.703  -8.289  1.00 54.57
ATOM   4467  CE2 TYR B 984       9.902   8.353  -8.361  1.00 55.09
ATOM   4468  CZ  TYR B 984       9.106   9.405  -7.952  1.00 54.72
ATOM   4469  OH  TYR B 984       7.984   9.146  -7.207  1.00 56.77
ATOM   4470  N   LEU B 985      15.996  11.157  -9.878  1.00 46.87
ATOM   4471  CA  LEU B 985      17.341  11.160 -10.459  1.00 46.02
ATOM   4472  C   LEU B 985      18.272  11.936  -9.519  1.00 46.87
ATOM   4473  O   LEU B 985      17.927  13.029  -9.063  1.00 45.27
ATOM   4474  CB  LEU B 985      17.344  11.812 -11.845  1.00 44.28
ATOM   4475  CG  LEU B 985      16.651  11.099 -13.001  1.00 43.30
ATOM   4476  CD1 LEU B 985      17.075  11.770 -14.289  1.00 43.28
ATOM   4477  CD2 LEU B 985      17.024   9.617 -13.037  1.00 43.77
ATOM   4478  N   VAL B 986      19.443  11.372  -9.226  1.00 46.59
ATOM   4479  CA  VAL B 986      20.381  12.023  -8.317  1.00 47.28
ATOM   4480  C   VAL B 986      21.628  12.479  -9.045  1.00 48.95
ATOM   4481  O   VAL B 986      22.479  11.675  -9.419  1.00 50.35
ATOM   4482  CB  VAL B 986      20.809  11.087  -7.179  1.00 49.66
ATOM   4483  CG1 VAL B 986      21.654  11.863  -6.171  1.00 48.82
ATOM   4484  CG2 VAL B 986      19.586  10.484  -6.507  1.00 48.62
ATOM   4485  N   ILE B 987      21.742  13.786  -9.214  1.00 49.22
ATOM   4486  CA  ILE B 987      22.854  14.377  -9.927  1.00 50.44
ATOM   4487  C   ILE B 987      23.496  15.472  -9.084  1.00 53.00
```

```
ATOM   4488  O   ILE B 987      22.797  16.347  -8.568  1.00 53.10
ATOM   4489  CB  ILE B 987      22.341  14.991 -11.246  1.00 49.77
ATOM   4490  CG1 ILE B 987      21.671  13.902 -12.087  1.00 50.87
ATOM   4491  CG2 ILE B 987      23.465  15.666 -11.995  1.00 48.64
ATOM   4492  CD1 ILE B 987      20.856  14.444 -13.253  1.00 51.02
ATOM   4493  N   GLN B 988      24.820  15.427  -8.946  1.00 55.17
ATOM   4494  CA  GLN B 988      25.537  16.446  -8.185  1.00 56.54
ATOM   4495  C   GLN B 988      25.166  17.807  -8.757  1.00 58.14
ATOM   4496  O   GLN B 988      25.094  17.971  -9.975  1.00 57.08
ATOM   4497  CB  GLN B 988      27.047  16.245  -8.300  1.00 57.24
ATOM   4498  CG  GLN B 988      27.612  15.195  -7.370  1.00 58.82
ATOM   4499  CD  GLN B 988      29.129  15.143  -7.409  1.00 60.42
ATOM   4500  OE1 GLN B 988      29.725  14.831  -8.441  1.00 63.50
ATOM   4501  NE2 GLN B 988      29.763  15.448  -6.282  1.00 62.41
ATOM   4502  N   GLY B 989      24.951  18.784  -7.879  1.00 59.86
ATOM   4503  CA  GLY B 989      24.562  20.106  -8.332  1.00 62.53
ATOM   4504  C   GLY B 989      23.067  20.003  -8.486  1.00 64.69
ATOM   4505  O   GLY B 989      22.426  19.366  -7.661  1.00 65.23
ATOM   4506  N   ASP B 990      22.494  20.611  -9.516  1.00 67.44
ATOM   4507  CA  ASP B 990      21.053  20.475  -9.704  1.00 70.60
ATOM   4508  C   ASP B 990      20.352  20.808  -8.377  1.00 72.92
ATOM   4509  O   ASP B 990      19.373  20.165  -7.996  1.00 73.02
ATOM   4510  CB  ASP B 990      20.764  19.019 -10.136  1.00 68.29
ATOM   4511  CG  ASP B 990      19.376  18.821 -10.727  1.00 65.16
ATOM   4512  OD1 ASP B 990      18.904  19.688 -11.493  1.00 64.82
ATOM   4513  OD2 ASP B 990      18.764  17.771 -10.433  1.00 61.33
ATOM   4514  N   ALA B 991      20.862  21.814  -7.675  1.00 75.66
ATOM   4515  CA  ALA B 991      20.275  22.219  -6.399  1.00 79.01
ATOM   4516  C   ALA B 991      19.048  23.107  -6.615  1.00 80.54
ATOM   4517  O   ALA B 991      17.965  22.739  -6.100  1.00 81.75
ATOM   4518  CB  ALA B 991      21.317  22.948  -5.537  1.00 77.93
ATOM   4519  OXT ALA B 991      19.180  24.153  -7.295  1.00 81.39
ATOM   4520  F1  LIG C   1     -21.453  16.649  -0.604  1.00 65.92
ATOM   4521  C2  LIG C   1     -21.069  17.936  -0.472  1.00 62.88
ATOM   4522  C3  LIG C   1     -19.922  18.287   0.383  1.00 60.99
ATOM   4523  C4  LIG C   1     -19.435  19.703   0.395  1.00 60.35
ATOM   4524  C5  LIG C   1     -20.135  20.740  -0.395  1.00 61.20
ATOM   4525  C6  LIG C   1     -21.331  20.391  -1.193  1.00 63.29
ATOM   4526  C7  LIG C   1     -21.800  18.979  -1.237  1.00 63.70
ATOM   4527  C8  LIG C   1     -18.188  20.151   1.138  1.00 58.87
ATOM   4528  O9  LIG C   1     -17.171  19.172   1.348  1.00 56.77
ATOM   4529  C10 LIG C   1     -16.358  18.640   0.332  1.00 55.56
ATOM   4530  C11 LIG C   1     -15.952  17.241   0.543  1.00 56.41
ATOM   4531  C12 LIG C   1     -15.101  16.562  -0.402  1.00 54.33
ATOM   4532  C13 LIG C   1     -14.603  17.275  -1.616  1.00 53.77
```

```
ATOM   4533  C14 LIG C   1     -15.012  18.688  -1.848  1.00 55.54
ATOM   4534  C15 LIG C   1     -15.913  19.352  -0.900  1.00 54.37
ATOM   4535  N16 LIG C   1     -13.762  16.701  -2.549  1.00 49.69
ATOM   4536  C17 LIG C   1     -13.714  15.438  -3.082  1.00 50.51
ATOM   4537  N18 LIG C   1     -14.809  14.489  -2.937  1.00 49.27
ATOM   4538  C19 LIG C   1     -14.740  13.219  -3.533  1.00 49.13
ATOM   4539  N20 LIG C   1     -13.631  12.866  -4.316  1.00 48.53
ATOM   4540  C21 LIG C   1     -12.558  13.784  -4.480  1.00 50.01
ATOM   4541  C22 LIG C   1     -12.550  15.113  -3.834  1.00 50.59
ATOM   4542  S23 LIG C   1     -11.201  16.018  -4.243  1.00 54.32
ATOM   4543  C24 LIG C   1     -10.572  14.794  -5.310  1.00 54.73
ATOM   4544  C25 LIG C   1     -11.377  13.652  -5.309  1.00 52.56
ATOM   4545  CL2 LIG C   1     -16.406  16.290   1.907  1.00 58.80
ATOM   4546  C27 LIG C   1      -8.858  16.177  -6.594  1.00 59.22
ATOM   4547  C26 LIG C   1      -9.449  14.847  -6.122  1.00 55.07
ATOM   4548  F1  LIG D   1      10.853  15.135 -41.543  1.00 58.61
ATOM   4549  C2  LIG D   1      11.037  13.839 -41.713  1.00 54.55
ATOM   4550  C3  LIG D   1      12.223  13.471 -42.454  1.00 54.59
ATOM   4551  C4  LIG D   1      12.685  12.058 -42.421  1.00 55.40
ATOM   4552  C5  LIG D   1      11.870  11.031 -41.722  1.00 55.68
ATOM   4553  C6  LIG D   1      10.584  11.399 -41.086  1.00 55.06
ATOM   4554  C7  LIG D   1      10.166  12.828 -41.075  1.00 55.50
ATOM   4555  C8  LIG D   1      14.013  11.667 -43.046  1.00 55.59
ATOM   4556  O9  LIG D   1      14.925  12.754 -43.284  1.00 54.46
ATOM   4557  C10 LIG D   1      15.752  13.298 -42.283  1.00 54.12
ATOM   4558  C11 LIG D   1      16.205  14.668 -42.540  1.00 54.63
ATOM   4559  C12 LIG D   1      17.138  15.313 -41.638  1.00 54.53
ATOM   4560  C13 LIG D   1      17.592  14.617 -40.390  1.00 54.63
ATOM   4561  C14 LIG D   1      17.151  13.224 -40.122  1.00 54.98
ATOM   4562  C15 LIG D   1      16.212  12.590 -41.043  1.00 53.54
ATOM   4563  N16 LIG D   1      18.380  15.217 -39.444  1.00 52.13
ATOM   4564  C17 LIG D   1      18.311  16.478 -38.879  1.00 52.92
ATOM   4565  N18 LIG D   1      17.153  17.343 -38.997  1.00 52.67
ATOM   4566  C19 LIG D   1      17.111  18.603 -38.359  1.00 52.27
ATOM   4567  N20 LIG D   1      18.197  19.019 -37.573  1.00 52.85
ATOM   4568  C21 LIG D   1      19.370  18.189 -37.471  1.00 53.46
ATOM   4569  C22 LIG D   1      19.449  16.879 -38.137  1.00 52.71
ATOM   4570  S23 LIG D   1      20.838  16.039 -37.751  1.00 55.09
ATOM   4571  C24 LIG D   1      21.417  17.235 -36.656  1.00 55.61
ATOM   4572  C25 LIG D   1      20.602  18.381 -36.703  1.00 54.95
ATOM   4573  CL2 LIG D   1      15.733  15.611 -43.921  1.00 56.18
ATOM   4574  C27 LIG D   1      23.036  15.744 -35.342  1.00 59.16
ATOM   4575  C26 LIG D   1      22.474  17.108 -35.765  1.00 54.82
ATOM   4576  O   HOH E   1      -7.599   8.623 -13.123  1.00 62.46
ATOM   4577  O   HOH E   2      24.517  23.513 -28.035  1.00 64.27
```

ATOM	4578	O	HOH E	3	-20.296	13.666	15.285	1.00	63.01
ATOM	4579	O	HOH E	4	-22.374	8.176	-7.192	1.00	49.42
ATOM	4580	O	HOH E	5	-29.264	30.402	-15.340	1.00	37.27
ATOM	4581	O	HOH E	6	-15.548	26.298	-3.002	1.00	60.28
ATOM	4582	O	HOH E	7	-16.488	46.164	-1.672	1.00	37.96
ATOM	4583	O	HOH E	8	-23.337	42.864	-22.019	1.00	54.63
ATOM	4584	O	HOH E	9	11.610	18.211	-56.805	1.00	64.90
ATOM	4585	O	HOH E	10	16.106	5.158	-39.459	1.00	71.20
ATOM	4586	O	HOH E	11	24.422	-1.900	-32.376	1.00	37.06
ATOM	4587	O	HOH E	12	18.940	-3.777	-26.629	1.00	37.73
ATOM	4588	O	HOH E	13	2.846	1.640	-26.716	1.00	48.90
ATOM	4589	O	HOH E	14	22.115	6.710	-30.625	1.00	46.15
ATOM	4590	O	HOH E	15	27.166	-0.416	-20.681	1.00	52.66
ATOM	4591	O	HOH E	16	27.370	0.625	-28.338	1.00	48.54
ATOM	4592	O	HOH E	17	8.879	-10.943	-20.472	1.00	43.79
ATOM	4593	O	HOH E	18	22.979	20.646	-12.884	1.00	55.83
ATOM	4594	O	HOH E	19	-23.835	38.304	-2.575	1.00	46.63
ATOM	4595	O	HOH E	20	3.858	19.802	-44.299	1.00	51.25
ATOM	4596	O	HOH E	21	6.565	20.312	-34.549	1.00	67.07
ATOM	4597	O	HOH E	22	6.762	22.561	-32.466	1.00	63.76
ATOM	4598	O	HOH E	23	17.087	2.388	-32.802	1.00	50.29
ATOM	4599	O	HOH E	24	19.085	-5.539	-28.680	1.00	47.97
ATOM	4600	O	HOH E	25	8.303	-6.214	-39.578	1.00	53.88
ATOM	4601	O	HOH E	26	24.363	7.903	-14.629	1.00	43.74
ATOM	4602	O	HOH E	27	-27.032	11.186	2.400	1.00	74.22
ATOM	4603	O	HOH E	28	-12.942	20.542	-5.335	1.00	44.65
ATOM	4604	O	HOH E	29	-7.825	34.064	-9.696	1.00	36.01
ATOM	4605	O	HOH E	30	6.161	13.446	-8.135	1.00	48.06
ATOM	4606	O	HOH E	31	4.895	21.272	-54.439	1.00	37.34
ATOM	4607	O	HOH E	32	14.560	16.150	-38.934	1.00	49.73
ATOM	4608	O	HOH E	33	-17.191	16.196	-2.787	1.00	49.94
ATOM	4609	O	HOH E	34	-12.431	16.753	-33.087	1.00	50.01
ATOM	4610	O	HOH E	35	19.316	15.273	-8.990	1.00	41.76
ATOM	4611	O	HOH E	36	22.919	-2.802	-12.770	1.00	32.09
ATOM	4612	O	HOH E	37	-20.465	42.538	-22.926	1.00	48.88
ATOM	4613	O	HOH E	38	24.551	-2.864	-35.433	1.00	38.92
ATOM	4614	O	HOH E	39	10.469	2.554	-40.581	1.00	54.18
ATOM	4615	O	HOH E	40	4.881	19.023	-24.625	1.00	58.60
ATOM	4616	O	HOH E	41	18.317	10.202	-53.601	1.00	71.11
ATOM	4617	O	HOH E	42	-13.865	22.064	10.271	1.00	57.28
ATOM	4618	O	HOH E	43	-35.587	21.497	3.030	1.00	36.88
ATOM	4619	O	HOH E	44	-26.803	14.899	-5.791	1.00	40.87
ATOM	4620	O	HOH E	45	-24.968	8.964	-9.528	1.00	60.43
ATOM	4621	O	HOH E	46	-18.782	34.826	-10.499	1.00	37.91
ATOM	4622	O	HOH E	47	-15.030	29.928	-8.619	1.00	52.85

```
ATOM   4623  O   HOH E  48     -19.234  30.472  -9.478  1.00 49.50
ATOM   4624  O   HOH E  49     -10.976  11.240  12.729  1.00 52.40
ATOM   4625  O   HOH E  50      16.214  -4.944 -38.622  1.00 53.39
ATOM   4626  O   HOH E  51     -14.354  32.711  -8.242  1.00 47.04
ATOM   4627  O   HOH E  52     -13.127  35.963 -19.946  1.00 44.74
ATOM   4628  O   HOH E  53     -26.260  30.450 -26.299  1.00 46.29
ATOM   4629  O   HOH E  54       9.344  23.549 -34.825  1.00 60.48
ATOM   4630  O   HOH E  55      12.830   1.506 -32.483  1.00 44.17
END
```

References

1. Johnson, L.N., Noble, M.E.M & Owen, D.J. (1996). Active and inactive protein kinases: structural basis for regulation. *Cell* **85**, 149-158.
2. Cox, S., Radzio-Andzelm, E. & Taylor, S.S. (1994). Domain movements in protein kinases. *Curr. Opin. Struct. Biol.* **4**, 893-901.
3. Schindler, T., Bornmann, W., Pellicena, P., Miller, W. T., Clarkson, B., Kuriyan, J.(2000). Structural Mechanism for Sti-571 Inhibition of Abelson Tyrosine Kinase. *Science* **289**, 1857-9.
4. Knighton, D.R., *et al.*, & Sowadski, J.M. (1991). Crystal structure of the catalytic subunit of cyclic adenosine monophosphate-dependent protein kinase. *Science* **253**, 407-413.
5. Mohammadi, M., Schlessinger, J. & Hubbard, S.R. (1996). Structure of the FGF receptor tyrosine kinase domain reveals a novel autoinhibitory mechanism. *Cell* **86**, 577-87.
6. Wybenga-Groot, L.E., Baskin, B., Ong, S.H., Tong, J., Pawson, T. & Sicheri, F. (2001). Structural Basis for Autoinhibition of the EphB2 Receptor Tyrosine Kinase by the Unphosphorylated Juxtamembrane Region. *Cell* **106**, 745-757.
7. Hubbard, S.R. (1997). Crystal structure of the activated insulin receptor tyrosine kinase in complex with peptide substrate and ATP analog. *Embo J.* **16**, 5572-5581.

8. Hubbard, S.R., Wei, L., Ellis, L. & Hendrickson, W.A. (1994). Crystal structure of the tyrosine kinase domain of the human insulin receptor. *Nature* **372**, 746-754.

9. McTigue,M.A., *et al.*, & Appelt,K. (1999). Crystal structure of the kinase domain of human vascular endothelial growth factor receptor 2: a key enzyme in angiogenesis. *Structure* **7**, 319-330.

10. Xu, W., Doshi, A., Lei, M., Eck, M.J. & Harrison SC (1999) Crystal structures of c-Src reveal features of its autoinhibitory mechanism. *Mol. Cell* **5**, 629-38.